

Optimizing two-qubit gates for ultracold atoms using Fermi-Hubbard models

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Ultracold atoms trapped in optical lattices have emerged as a scalable and promising platform for quantum simulation and computation; however, gate speeds remain a significant limitation for practical applications. In this work, we employ quantum optimal control to design fast, collision-based two-qubit gates within a superlattice based on a Fermi-Hubbard description, reaching errors in the range 10^{-3} for realistic parameters. Numerically optimizing the lattice depths and the scattering length, we effectively manipulate hopping and interaction strengths intrinsic to the Fermi-Hubbard model. Our results provide five times shorter gate durations by allowing for higher energy bands in the optimization, suggesting that standard modeling with a two-band Fermi-Hubbard model is insufficient for describing the dynamics of fast gates, and we find that four to six bands are required. Additionally, we achieve nonadiabatic gates by employing time-dependent lattice depths rather than using only fixed depths. The optimized control pulses not only maintain high efficacy in the presence of laser-intensity and phase noise but also result in negligible interwell couplings.

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I. INTRODUCTION

After decades of research, many physical systems have been proven capable of serving as platforms for quantum information processing, including superconducting circuits [1–3], trapped ions [4–7], ultracold atoms [8–10], photons [11–14], defects in solids [15,16], and quantum dots [17–19]. Among these promising systems, neutral atoms have emerged over the last decade as a leading platform for quantum simulation and computing [20–23]. These atoms are typically trapped in optical tweezers or lattices, allowing for the arrangement of hundreds of atoms in arbitrary geometries. Quantum information is generally encoded in the internal states of the atoms, with two-qubit gates using atomic interactions [24–28]. These interactions can be short ranged, such as van der Waals interactions [29], or they can have considerably longer ranges, such as dipole-dipole interactions [30]. One successful approach is excitation to Rydberg states, which facilitates strong and controllable interactions, enabling the study of many-body

dynamics and the execution of quantum logic operations [31,32].

An alternative approach to Rydberg atoms is to work with ground-state atoms trapped in optical lattices or superlattices [33–43]. A superlattice is formed by superimposing at least two optical lattices with different wavelengths and has multiple double-well structures [44,45]. These systems naturally realize the Hubbard model [8, 46]. Neutral atoms in an optical lattice can be arranged in arbitrary configurations using efficient atom-transport mechanisms [47–49]. The exchange of atoms and their entanglement is generated through controlled collisions between the atoms, enabling the implementation of essential quantum gates such as SWAP and $\sqrt{\text{SWAP}}$ [50,51]. Combined with single-qubit rotations, these gates constitute a universal gate set for quantum simulation and computation [52,53]. The collision interactions are tuned by adjusting the barrier height of the double well and its scattering length. To ensure that the system adheres to Hubbard-model dynamics, the exchange interactions must be controlled to prevent atom excitations [54,55]. Most directly, this is achieved by adiabatically changing the barrier heights [52]; however, this approach results in slower gates, which can reduce the coherence time and affect longer circuits in quantum simulation and computation.

Faster and more efficient gates can be achieved using optimal control methods, which have become an integral part of quantum computing, quantum simulation, and

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quantum information processing [56–60]. The efficiency of quantum operations is increased by shaping their driving fields using analytical and numerical techniques. Analytical methods are usually only applicable to smaller systems requiring a detailed understanding of their dynamics [61–71], while the results of Refs. [67,72–75] are relevant for the analytical aspects of our work. In contrast, numerical methods can often be implemented with partial (or no) knowledge of the system dynamics, and they can depend on the system and rely on open- or closed-loop approaches (i.e., without or with feedback, respectively) [76–91].

In this article, we use open-loop optimal control techniques to develop fast SWAP and $\sqrt{\text{SWAP}}$ gates for fermionic ^6Li atoms trapped in a superlattice. We describe our system with a Fermi-Hubbard model using realistic experimental parameters [37,44,45]. To this end, we optimize the lattice depths and s-wave scattering parameter to achieve high-fidelity state transfer from an initial state $\Psi_0 = |\uparrow\downarrow\rangle$ to target states $\Psi_{\text{SWAP}} = |\downarrow\uparrow\rangle$ and $\Psi_{\sqrt{\text{SWAP}}} := [(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$ and eventually find high-fidelity gates. Our study reveals that the two-band Fermi-Hubbard model is insufficient for explaining the dynamics of these fast gates (see Result 3).

The key idea of our fast gates is to extend the Fermi-Hubbard model to include the higher-energy bands (see Sec. IV A). Using realistic experimental parameters, we numerically demonstrate that the control duration for transferring state Ψ_0 to Ψ_{SWAP} with fidelity 0.999 is as short as 0.08 ms, and it is 0.12 ms for transferring Ψ_0 to $\Psi_{\sqrt{\text{SWAP}}}$ with fidelity 0.995, which is five times shorter than typical experimental state-transfer times [44,45] (see Result 4). These fidelities can be further improved, and we show that they are mainly limited by the available laser power. We also detail that these optimized controls are robust against intensity and phase noise and result in minimal interwell tunneling (see Result 5), which enables improved coherence times of 460 Rabi oscillations, compared to the value of 33 Rabi oscillations reported in a recent experimental study [44]. Moreover, in Sec. VI, we analyze how our gates perform when they are applied to error states with three and four atoms in a double well, which provides a more complete understanding of the system dynamics under various experimentally possible scenarios. Lastly, in Sec. VIII, we show that for fast gates, the initial states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ can excite to higher levels, and this can be minimized with a full gate optimization. The full gate optimization yields a SWAP gate with a fidelity of 0.997 in 0.10 ms and a $\sqrt{\text{SWAP}}$ gate with a fidelity of 0.993 for a gate duration of 0.16 ms (see Result 6).

Our results initially arise from analytical and numerical optimizations using a two-band Fermi-Hubbard model (see Results 1 and 2), where the gradients for the numerical optimization are computed based on a particularly effective spline-fit approach (see Sec. III B). For higher-band Fermi-Hubbard models, the spline-fit approach is not

applicable in the presence of multiple hopping and interaction terms, and we instead develop an approach using an effective approximate analytical gradient in Appendix B. The performance of the different gradient approaches is compared in Appendix C. Thus, our work combines faster, robust two-qubit gates for ultracold atoms under realistic experimental conditions with methodological advances.

The structure of the remainder of this paper is as follows. In Sec. II, we define the Hamiltonian for the superlattice potential, introduce the corresponding two-band Fermi-Hubbard model, and explain the objective of the quantum control tasks. We then optimize the SWAP and $\sqrt{\text{SWAP}}$ gates using both analytical and numerical techniques in Sec. III. In Sec. IV, we explore the impact of higher energy bands on the optimized fast gates and demonstrate the limitations of the two-band Fermi-Hubbard model. Next, in Sec. V, we present the optimization of the SWAP and $\sqrt{\text{SWAP}}$ gates using the higher-band Fermi-Hubbard model. In Sec. VI, we investigate the dynamics of more than two atoms in a double well under the optimal control pulses, and we analyze the robustness of the optimized control pulses in Sec. VII. We perform a full gate optimization to minimize the gate error for different basis states in Sec. VIII. In Sec. IX, we discuss the effect of high interaction strength on $\sqrt{\text{SWAP}}$ transfer. Finally, we summarize our conclusions in Sec. X. The raw data files from the simulations performed for this work are provided in Ref. [92].

II. MODEL AND OBJECTIVE

A. Model

We consider a double-well potential, the barrier heights of which can be controlled dynamically [44,45], as

$$V(\mathbf{r}, t) = V_s(t) \cos^2(k_s x + \varphi(t)) - V_\ell(t) \cos^2(k_\ell x) - V_y \cos^2(k_y y) - V_z \cos^2(k_z z), \quad (1)$$

where $\mathbf{r} = (x, y, z)$. In the x direction, a superlattice or a double-well potential [see Fig. 1] is created by standing waves from two tilted lasers with a short wavelength of $\lambda_s = 532$ nm and two lasers with a long wavelength of $\lambda_\ell = 1064$ nm. The wave vectors of the lattice are then given by $k_b = 2\pi/\lambda_b \sin(26.7^\circ/2)$, with $b \in \{s, \ell\}$, where 26.7° is the angle between the tilted lasers constructing the lattice, chosen for the particular geometry of the experimental system [44]. Here, $V_s(t)$ and $V_\ell(t)$ respectively denote the tunable lattice depths for the short and long lattice, where the short lattice is blue detuned (repulsive) and the long lattice is red detuned (attractive). The tunable relative phase between the short and long lattice is given by $\varphi(t)$. We consider optical lattices with constant lattice depths $V_y = 45E_{ry}$ and $V_z = 45E_{rz}$ in the y and z directions, respectively, expressed in units of their respective recoil energies $E_{ry} = \hbar^2 k_y^2 / (2m)$ and $E_{rz} = \hbar^2 k_z^2 / (2m)$.

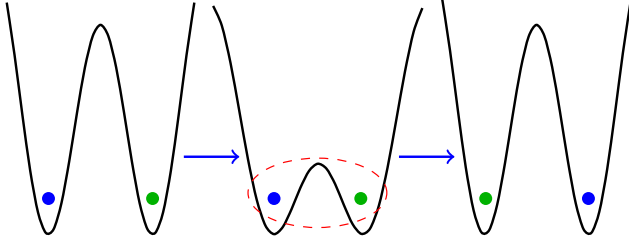


FIG. 1. Collision gate in a double well. A double well is initialized with two ^6Li atoms. The green atom on the right is in the state $|\uparrow\rangle$ and the blue atom on the left is in the state $|\downarrow\rangle$, which yields the state $|\uparrow\downarrow\rangle$. The barrier inside the double well is lowered in a controlled way to allow the two atoms to interact. This results in a SWAP or $\sqrt{\text{SWAP}}$ gate between the two atoms. The SWAP gate exchanges the spins and prepares the state $|\downarrow\uparrow\rangle$, while the $\sqrt{\text{SWAP}}$ gate prepares the state $[(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$.

Following the experimental work of Ref. [44], we initialize the double well with two fermionic ^6Li atoms, where one atom is in the spin-up state and the other is in the spin-down state, as shown in Fig. 1. We model the system of two atoms based on the Hamiltonian

$$H_1(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t), \quad (2)$$

$$H_2(\mathbf{r}_1, \mathbf{r}_2, t) = \sum_{j=1}^2 H_1(\mathbf{r}_j, t) + U_{3D}(\mathbf{r}_1, \mathbf{r}_2), \quad (3)$$

where m is the mass of the ^6Li atoms and H_1 is the single-atom Hamiltonian. Here, the pseudointeraction potential $U_{3D}(\mathbf{r}_1, \mathbf{r}_2)$ between the atoms is defined as

$$U_{3D}(\mathbf{r}_1, \mathbf{r}_2) = \frac{4\pi\hbar^2}{m}a\delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (4)$$

and a denotes the characteristic scattering length. In an experiment, a is tuned by changing the magnetic field, giving Feshbach resonances [93]. Since the optical potential of Eq. (1) separates into the three spatial components, one can independently solve them in the noninteracting case. Thus, we can concentrate only on the x -direction dependence of Eqs. (2) and (3) for our calculations. For interacting particles, this argument holds approximately if one assumes that either the control pulses remain in the adiabatic regime (without excitations in the y and z directions) or that the optical potential in the y and z directions is strong enough such that the interaction energy is low enough to not excite the atoms in those dimensions. A mixture of both assumptions is valid for our work. We write the single-atom Hamiltonian of Eq. (2) in Fourier space as

$$\tilde{H}_1(q) = \frac{\hbar^2}{2m}q^2 + \tilde{V}(q), \quad (5)$$

where $\tilde{V}(q)$ is the Fourier expansion of the lattice potential with quasimomentum q . We assume a lattice with L sites and discretized values for the momenta $q = fk_s + k$, with $f \in \mathbb{Z}$, $k = k_s(2n + 1 - L)/2L$, and $n \in [0, L - 1]$ in the first Brillouin zone.

From Bloch's theorem, the eigenfunctions of $\tilde{H}_1(q)$ can be written in the form

$$\Phi_{b,k}(x) = e^{ikx/\hbar}\phi_{b,k}(x),$$

$$\text{where } \phi_{b,k}(x) = \sum_m C_{m,b,k} e^{ifk_s x}.$$

Here, $C_{m,b,k}$ are coefficients obtained by solving for the eigenstates of Eq. (5), b denotes the band index, and $\phi_{b,k}(x)$ are periodic functions with periodicity $d = \lambda_\ell/2$, i.e., $\phi_{b,k}(x) = \phi_{b,k}(x + d)$. The Bloch states $\Phi_{b,k}(x)$ are localized in momentum space but completely delocalized in real space. Equivalently, we can define a set of basis states called Wannier states, which are localized in real space [94–96]. We choose the Wannier states as the basis in which our system is specified. This choice is motivated by the assumption that the wave function of the atoms is localized on one side of the double well and close to the ground state of the optical lattice. Under these assumptions, the wave functions can be described with only a few Wannier states. We can calculate Wannier functions w_b based on the idea that these states are defined as the eigenstates of the position operator X such that

$$X_b w_b(x - x_0) = x_0 w_b(x - x_0).$$

For this, we write the position operator

$$X_{b,k',k} = \int \Phi_{b,k'}^*(x) x \Phi_{b,k}(x) dx$$

in terms of the Bloch state basis $\Phi_{b,k}(x)$. The Wannier function $w_b(x - x_0)$ in band b at position $x - x_0$ in the x direction is defined as

$$w_b(x - x_0) = \frac{1}{\sqrt{L}} \sum_k e^{-i(kx_0 + \chi_k)} \Phi_{b,k}(x),$$

with a momentum-dependent phase χ_k , which is given by the condition that the Wannier states are the eigenstates of the position operator X . Note that even if the Wannier states build an orthonormal basis, they are not the eigenstates of the Hamiltonian. Nevertheless, the stronger the optical potential becomes, the flatter the bands are in k , and as a result, the Wannier states match more closely with the eigenstate of the Hamiltonian. For a double-well system as shown in Fig. 2, one can always take a linear combination of two bands ($2p$ and $2p + 1$) to construct the left w_L and right w_R basis states of the level p . For that, one only needs to apply the condition that the Wannier states

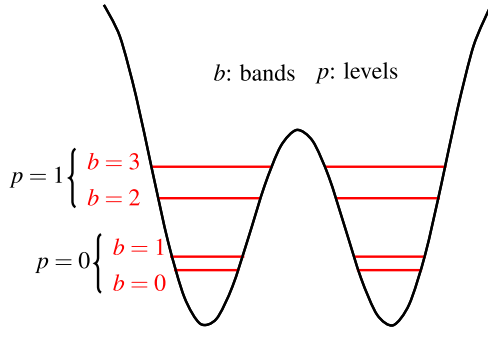


FIG. 2. Level scheme of the multiband Fermi-Hubbard model for one double well of the superlattice potential described by Eq. (1). The bands appear in pairs, with each pair corresponding to one level p of the model. For instance, four bands form two levels, where the zeroth ($b = 0$) and first ($b = 1$) bands form level $p = 0$, and the second ($b = 2$) and third ($b = 3$) bands form level $p = 1$.

w_L and w_R are still the eigenstates of the position operator X . Examples of Wannier states are shown in Fig. 3.

Instead of simulating the real-space Hamiltonian of Eq. (3), we can also describe fermionic atoms trapped in the optical lattices with the Fermi-Hubbard model [97,98] as

$$\hat{H} = -J \sum_{i \neq j, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (6)$$

where the operator $c_{i\sigma}^\dagger$ (or $c_{i\sigma}$) creates (or annihilates) an atom in the spin state $\sigma \in \{\uparrow, \downarrow\}$ at lattice site i . The operators $c_{i\sigma}^\dagger$ and $c_{j\sigma'}$ have the anticommutation relation

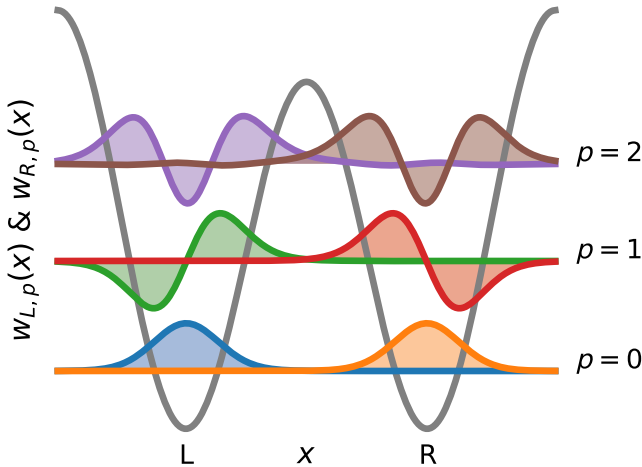


FIG. 3. The Wannier states $w_{L,p}$ and $w_{R,p}$ in the left and the right bases of the first three levels $p = 0$, $p = 1$, and $p = 2$ for the corresponding optical potential in the x direction. Each level p is constructed from a linear combination of the two bands $b = 2p$ and $b = 2p + 1$, as also shown in Fig. 2.

$\{c_{i\sigma}^\dagger, c_{j\sigma'}\} = \delta_{ij} \delta_{\sigma\sigma'}$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator. The first term represents hopping between site i and j of the lattice with amplitude J . The second term describes an interaction of strength U between two atoms of opposite spins sitting on the same site i of the lattice. The model of Eq. (6) is sufficient to describe the atoms in an optical lattice with periodic single wells; however, for a superlattice with periodic double wells and relevant depth, the gap between the two lowest-energy bands becomes very small inside each double well, as shown in Figs. 1 and 2. Therefore, we extend the one-band Fermi-Hubbard model to a two-band model for describing the dynamics of the double well. We assume that all the higher bands ($b > 1$), as shown in Fig. 2, are still separated by a large energy gap and the two-band model sufficiently describes the system.

The two-band Fermi-Hubbard model for two atoms in an individual double well [44,45] is given by

$$\hat{H} = -J \sum_{\sigma} (c_{L\sigma}^\dagger c_{R\sigma} + \text{H.c.}) + U \sum_{\alpha=L,R} n_{\alpha\uparrow} n_{\alpha\downarrow}, \quad (7)$$

where $c_{L\sigma}^\dagger$ (or $c_{L\sigma}$) and $c_{R\sigma}^\dagger$ (or $c_{R\sigma}$) create (or annihilate) a fermion in spin state $\sigma \in \{\uparrow, \downarrow\}$ on the left (L) or the right (R) side of the double well, respectively. Equation (7) resembles Eq. (6), with the site index i replaced by the left (L) and right (R) side of the double well. The first term represents hopping between the left and the right sides of the double well with amplitude J . The second term describes an interaction of strength U between two atoms of opposite spins sitting on the same side of the double well. Throughout the paper, we work with a symmetric double well, i.e., $\varphi(t) = 0$ [see Eq. (1)]. Thus, U is identical for the left and right wells. The gates are based on the hopping and the onsite interaction of the atoms in the double well, which are given by

$$J = - \int w_R(x) H_1(x) w_L(x) dx, \quad (8)$$

$$U = \iint U_{3D}(\mathbf{r}_1, \mathbf{r}_2) w_\alpha^2(\mathbf{r}_1) w_\alpha^2(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \quad (9)$$

where U is assumed to be independent of $\alpha \in \{L, R\}$. The pseudointeraction potential $U_{3D}(\mathbf{r}_1, \mathbf{r}_2)$ is defined in Eq. (4), and $H_1(x)$ is the single-atom Hamiltonian from Eq. (2) in the x direction. The function $w_\alpha(\mathbf{r}) = w_\alpha(x) w_0(y) w_0(z)$ is the three-dimensional Wannier state, where $w_L(x)$ and $w_R(x)$ represent the states in the x direction on the left (L) and right (R) sides of the double well, respectively. The Wannier states of the lowest band in the y and the z directions are $w_0(y)$ and $w_0(z)$, respectively. As explained in Table I, the hopping strength J is calculated from the time-dependent lattice depths $V_s(t)$ and $V_\ell(t)$. The onsite interaction U depends on the constant scattering length a , along with the lattice depths $V_s(t)$ and

TABLE I. Different Fermi-Hubbard parameters and the corresponding tunable experimental parameters. There are two Fermi-Hubbard parameters: interaction strength U and hopping strength J . For the two-band Fermi-Hubbard model, J is time-dependently tuned using the lattice depths V_s and V_ℓ , whereas we assume that U is time independent and tuned by the scattering length a . The conversion relations between the experimental parameters and the Fermi-Hubbard parameters are given by Eqs. (8)–(9). For the higher-band model, we have multiple J_p values for different p levels of the double well, controlled by V_s and V_ℓ with Eq. (18). Similarly, we have multiple time-dependent $U_{mnop}^{\alpha\beta\gamma\delta}(t)$ tuned by a , V_s , and V_ℓ with Eq. (19), as detailed in Sec. IV A.

Model	Gate	Fermi-Hubbard parameters	Experimental parameters
Two band	SWAP	$J(t)$	$V_s(t), V_\ell(t)$
	$\sqrt{\text{SWAP}}$	$J(t)$	$V_s(t), V_\ell(t)$
		U	a
Higher band	SWAP	$J_p(t)$	$V_s(t), V_\ell(t)$
	$\sqrt{\text{SWAP}}$	$J_p(t)$	$V_s(t), V_\ell(t)$
		$U_{mnop}^{\alpha\beta\gamma\delta}(t)$	$a, V_s(t), V_\ell(t)$

$V_\ell(t)$. In the two-band description, U is almost independent of the change in the long-lattice depth V_ℓ , and it increases with increasing short-lattice depth V_s ; however, U can be tuned over a much larger range by changing a , V_y , and V_z compared to changing V_s [99]. As a simplification, for the two-band model, we assume that the change in the onsite interaction depends only on the change in the s-wave scattering with tunable constant scattering length a . We can calculate $J(t)$ and U from the experimental parameters V_s , V_ℓ , and a using Eqs. (8) and (9), respectively; however, the reverse calculation of the experimental parameters $V_s(t)$ and $V_\ell(t)$ from a given $J(t)$ is more problematic, as explained in Sec. III B.

B. Objective

The two-qubit gates for the fermionic system in the superlattice can be represented using the spin-nonconserving basis states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, where each state represents atoms on the left (L) and the right (R) side of the double well [51,52]. The state $|\uparrow\downarrow\rangle$ therefore describes the first atom in the left (L) well being in the spin-up state and the second atom in the right (R) well being in the spin-down state. In this basis, the total spin of the system is not conserved. The SWAP and $\sqrt{\text{SWAP}}$ gates are represented in this basis as

$$\text{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\sqrt{\text{SWAP}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & (1+i)/2 & (-1+i)/2 & 0 \\ 0 & (-1+i)/2 & (1+i)/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

In the two-band Fermi-Hubbard model, two fermionic atoms with spin up or down can only attain the states $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$, respectively, and they are hence fixed by Pauli's exclusion principle. Therefore, applying a SWAP or $\sqrt{\text{SWAP}}$ gate will not change their states. Therefore, we focus on the basis $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. From the symmetry of the Hamiltonian, a SWAP or $\sqrt{\text{SWAP}}$ gate will perform the same operation on $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, which means that any pulses transferring the state $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$ will also transfer $|\downarrow\uparrow\rangle$ to $|\uparrow\downarrow\rangle$. Hence, it is sufficient to optimize the transfer of the state

$$\Psi_0 := |\uparrow\downarrow\rangle \text{ to } \Psi_{\text{SWAP}} := |\downarrow\uparrow\rangle$$

using a time-dependent control $J(t)$ at $U = 0$ and later verify that this also transfers $|\downarrow\uparrow\rangle$ to $|\uparrow\downarrow\rangle$. Similarly, it is enough for the optimization of the $\sqrt{\text{SWAP}}$ gate to optimize the transfer of the state

$$\Psi_0 \text{ to } \Psi_{\sqrt{\text{SWAP}}} := [(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$$

using $J(t)$ and the time-independent control U . Therefore, we only need to solve a state-to-state transfer problem for obtaining the SWAP and $\sqrt{\text{SWAP}}$ gates in the two-band Fermi-Hubbard model.

With one atom in the spin-up state and a second one in the spin-down state, we can have four possible states $|D0\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|0D\rangle$, where D denotes double occupancy on the left or the right side of the double well. The states $|D0\rangle$ and $|0D\rangle$ are outside our two-qubit computational basis. Hence, our goal is to minimize the probability that the states $|D0\rangle$ and $|0D\rangle$ are observed at the end of the SWAP or $\sqrt{\text{SWAP}}$ gates. Additionally, the double well can accommodate up to four fermionic atoms, with two atoms in the spin-up state and two atoms in the spin-down state. One-atom states serve as single-qubit states; however, for two-qubit gates, states with three and four atoms are error states. Hence, we do not consider these error states in the optimization and only check the performance of our optimized pulses for these error states in Sec. VI.

III. OPTIMIZATION WITH A TWO-BAND FERMION-HUBBARD MODEL

As explained in Sec. II B, we aim to optimize the transfer from Ψ_0 to Ψ_{SWAP} or $\Psi_{\sqrt{\text{SWAP}}}$ by minimizing the population of the states $|D0\rangle$ and $|0D\rangle$. First, we optimize the hopping parameter $J(t)$ for the SWAP gate using analytical methods. Later, we compare our results with the numerical optimization in Sec. III B.

A. Analytical optimization

In this section, we study the problem of finding the time-optimal pulse sequence to perform the SWAP gate. In particular, we find the minimum time for transferring the state $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$ in the two-band Fermi-Hubbard model without any interaction, i.e., for $U = 0$. The interaction strength U can, in principle, be tuned to zero either by changing the internal atomic state to a noninteracting one or by tuning the magnetic field to set $a = 0$ [100,101]. The time-optimal pulse also transfers the state $|\downarrow\uparrow\rangle$ to $|\uparrow\downarrow\rangle$. Similar problems have been extensively studied in other systems [67,72–75]. The system Hamiltonian is given by

$$H'(t) = \begin{bmatrix} U & -J(t) & -J(t) & 0 \\ -J(t) & 0 & 0 & -J(t) \\ -J(t) & 0 & 0 & -J(t) \\ 0 & -J(t) & -J(t) & U \end{bmatrix} \quad (10)$$

in the basis corresponding to the basis states $|D0\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|0D\rangle$. We switch to a new basis $(|D0\rangle + |0D\rangle)/\sqrt{2}$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $(|D0\rangle - |0D\rangle)/\sqrt{2}$, which allows us to neglect the state $(|D0\rangle - |0D\rangle)/\sqrt{2}$ (in our analytical optimization) as it does not couple with the other states. Therefore, the time evolution with $\tilde{J}(t) = -\sqrt{2}J(t)$ and $U = 0$ is

$$i \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{bmatrix} 0 & 0 & \tilde{J}(t) \\ 0 & 0 & \tilde{J}(t) \\ \tilde{J}(t) & \tilde{J}(t) & 0 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad (11)$$

where x_1 , x_2 , and x_3 correspond to complex coefficients of the states $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $(|D0\rangle + |0D\rangle)/\sqrt{2}$, respectively. Thus, optimizing the SWAP gate reduces to finding $\tilde{J}(t)$ for evolving the system from $(1, 0, 0)^T$ to $(0, 1, 0)^T$. To obtain the time-optimal solution, we follow the standard approach [67,72–75], which is based on solving suitable Euler-Lagrange equations. The calculation is detailed in Appendix A, and it shows that the time-optimal $J(t)$ is a constant pulse. Other more direct approaches might be applicable in this particular case, but the calculations in Appendix A also prepare the ground for future work to explore analytical solutions beyond the considered two-band Fermi-Hubbard model.

Result 1. The time-optimal SWAP gate in the two-band Fermi-Hubbard model without any interaction (i.e., $U = 0$) is given by a constant pulse $J(t) = J_{\max}$, where $J_{\max}$ is the maximal experimentally possible hopping strength J . The minimum gate duration to transfer the state from $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$ or vice versa is given by $T = \pi/(2J_{\max})$. For $J_{\max} = 34.03$ kHz, we get $T = \pi/(2J_{\max}) = 0.046$ ms. The explicit form of the state evolution follows from Eq. (A6).

Remark 1. The state $|\uparrow\downarrow\rangle$ can only be transformed into $|\downarrow\uparrow\rangle$ using a real $J(t)$. The -1 phase of $|\downarrow\uparrow\rangle$ appears

ALGORITHM 1. Optimization of the SWAP and $\sqrt{\text{SWAP}}$ gates using the two-band model.

SWAP:

Input: $a = 0$

Optimization parameters: $V_s(t)$ and $V_\ell(t)$

Step 1: Define the SWAP-gate cost function $C_{\text{SWAP}} = 1 - |\langle \Psi_{\text{SWAP}} | \Psi(T) \rangle|^2$

Step 2: Minimize C_{SWAP} to find optimal V_s and V_ℓ using gradient-based optimization with the spline-fit method

Output: Optimized $V_s(t)$ and $V_\ell(t)$ for the SWAP gate

$\sqrt{\text{SWAP}}$:

Input: $V_s(t)$ and $V_\ell(t)$ from the SWAP gate

Optimization parameters: a

Step 1: Define the $\sqrt{\text{SWAP}}$ -gate cost function $C_{\sqrt{\text{SWAP}}} = 1 - |\langle \Psi_{\sqrt{\text{SWAP}}} | \Psi(T) \rangle|^2$

Step 2: Perform a one-dimensional search to minimize $C_{\sqrt{\text{SWAP}}}$ and optimize a

Output: Optimized a for the $\sqrt{\text{SWAP}}$ gate

since the Hamiltonian is written using the spin-ordered convention, where the creation operators are applied on the vacuum $|00\rangle$ in the order $c_{R\downarrow}^\dagger c_{L\downarrow}^\dagger c_{R\uparrow}^\dagger c_{L\uparrow}^\dagger$ and thus

$$\text{SWAP}' = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

We can also write the Hamiltonian using the site-ordered convention, where the creation operators are applied on the vacuum $|0\rangle$ in the order $c_{R\downarrow}^\dagger c_{R\uparrow}^\dagger c_{L\downarrow}^\dagger c_{L\uparrow}^\dagger$. The site-ordered convention gives the usual SWAP operation. One can apply the matrix $\text{diag}(1, -1, -1, 1)$ on SWAP' to get SWAP, which requires a phase change conditional on the spin parity. Optimizations performed in this work use the spin-ordered convention, but the results are easily adaptable to the site-ordered convention. Therefore, we neglect the phase of the target states for our numerical optimizations.

In the next section, we use a gradient-based numerical optimization to find the optimal $J(t)$ for the SWAP gate and compare it with the analytical result.

B. Numerical optimization

As explained in Sec. II A, the hopping parameter J is tuned by changing the lattice depths V_s and V_ℓ , while the interaction strength U is controlled by the constant scattering length a . The conversion relations between the experimental parameters and the Fermi-Hubbard parameters are given by Eqs. (8) and (9). To perform experiments with optimal control pulses, we need to convert the optimized J and U to the experimental parameters V_s , V_ℓ , and a ; however, reconstructing V_s and V_ℓ from J is nontrivial

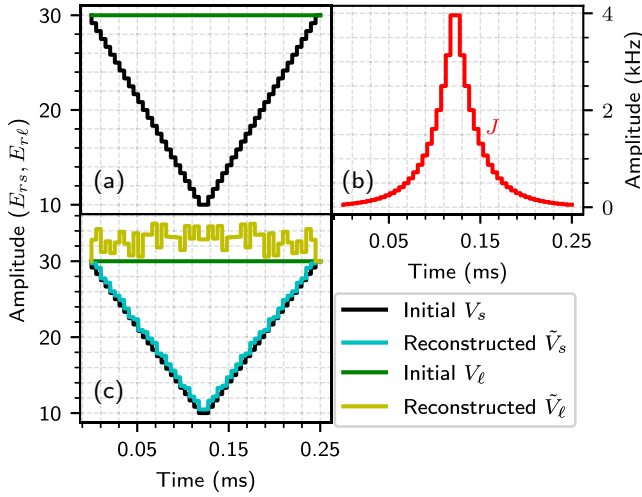


FIG. 4. Relations between (a) the lattice depths V_s and V_l in their respective recoil energies $E_{rs(\ell)} = \hbar^2 k_{s(\ell)}^2 / 2m$ and (b) the corresponding hopping strength J via Eq. (8). (c) The nonrecommended noisy reconstructions of V_s and V_l from the hopping strength J in (b) significantly differ from their initial values in (a). This is avoided by directly optimizing V_s and V_l , as detailed in Sec. III B.

and introduces noise. To test the reconstruction performance, we start with an initial set of V_s and V_l [shown in Fig. 4(a)], expressed in units of their respective recoil energies $E_{rs} = \hbar^2 k_s^2 / (2m)$ and $E_{rl} = \hbar^2 k_l^2 / (2m)$. These lattice depths generate an exponentially changing J , as shown in Fig. 4(b). We then attempt to reconstruct the initial lattice depths from J using a prestored data table of V_s , V_l , and J . As shown in Fig. 4(c), the reconstructed long-lattice depth $\tilde{V}_l$ does not match the initial V_l , and the back conversion also introduces noise to the reconstructed short-lattice depth $\tilde{V}_s$.

Remark 2. Optimizing J and converting it back to lattice depths V_s and V_l is not effective for obtaining smooth and realistic pulses. Therefore, for the remainder of this work, we directly optimize the experimental parameters V_s , V_l , and a to achieve the optimized SWAP and $\sqrt{\text{SWAP}}$ gates.

We can apply a gradient-based optimization technique known as GRAPE [76], which can also use Newton or quasi-Newton (Broyden-Fletcher-Goldfarb-Shanno) methods [80, 102–105] and can include different transfer functions [106, 107] to optimize V_s and V_l for the SWAP gate with $a = 0$. For the $\sqrt{\text{SWAP}}$ gate, we use the optimized V_s and V_l from the SWAP gate and conduct a one-dimensional search with the target state $\Psi_{\sqrt{\text{SWAP}}}$ to identify the optimal scattering length a for the $\sqrt{\text{SWAP}}$ gate. Algorithm 1 briefly explains the optimization steps for the SWAP and $\sqrt{\text{SWAP}}$ gates for a two-band Fermi-Hubbard model.

We need to calculate the gradients of the cost function with respect to V_s and V_l for the gradient-based optimization of the SWAP gate. For this, we can express the Hamiltonian of Eq. (11) as a control Hamiltonian given by

$$H(t) = J(t)H_J, \quad (12)$$

where H_J is constant in time and $U = 0$ for the SWAP gate. Our goal is now to transfer a quantum system from the given initial pure state $\Psi_{\text{ini}} = \Psi_0$ to the target pure state $\Psi_{\text{tar}} = \Psi_{\text{SWAP}}$ in time T by varying the control pulse $J(t)$ while minimizing the cost function

$$C = 1 - |\langle \Psi_{\text{tar}} | \Psi(T) \rangle|^2. \quad (13)$$

We divide the total control duration T into N_T equal steps of duration $\Delta t = T/N_T$, which results in a piecewise-constant $J(t)$. The time evolution of the quantum system during the j th time step is given by

$$\mathcal{U}_j = \exp[-i\Delta t J(j)H_J]. \quad (14)$$

The cost function (13) can be written as

$$C = 1 - |\langle \Psi_{\text{tar}} | \mathcal{U}_{N_T} \cdots \mathcal{U}_1 | \Psi_{\text{ini}} \rangle|^2. \quad (15)$$

To minimize C , at every iteration of the algorithm, we update the controls by

$$J(j) \rightarrow J(j) - \epsilon \frac{\delta C}{\delta J(j)},$$

where ϵ is a small unitless step matrix.

In our case, we now perform a change of controls from the experimental parameters $V_k \in \{V_s, V_l\}$ to the Fermi-Hubbard parameter J , where V_k and J are piecewise constant with N_T time steps. Hence, we follow the derivation in Ref. [105], where the product rule is applied to the gradient calculation, and one obtains

$$\frac{\delta C}{\delta V_k(j)} = \sum_{s=1}^{N_T} \frac{\delta J(s)}{\delta V_k(j)} \frac{\delta C}{\delta J(s)}.$$

The derivative $\delta C / \delta J(s)$ is calculated here with the help of the Fréchet-derivative method [108] using the PYTHON package SCIPY [109]. We use a spline-fit method for calculating the Fermi-Hubbard parameter J and its gradient with respect to the lattice depths at each time step and every optimization iteration, i.e., $\delta J(s) / \delta V_k(j)$. For this, we create a grid of 100×100 pairs (V_s, V_l) , where V_s ranges from $2E_{rs}$ to $30E_{rs}$ and V_l ranges from $30E_{rl}$ to $50E_{rl}$. We calculate and store the value of J for each point on the grid. Using the prestored dataset of triples (V_s, V_l, J) , we fit a bivariate spline function of degree three using SCIPY [109]

and calculate the fit coefficients. Finally, using these coefficients, we can calculate the values of J and $\delta J/\delta V_k$ for new values of $V_k \in \{V_s, V_\ell\}$ during the optimization. To obtain a good fit, we should have enough prestored dataset of triples (V_s, V_ℓ, J) , and we see that a grid of 100×100 is sufficient. As explained in Appendix C, the spline-fit method is computationally efficient and enables faster optimization compared to calculating J and $\delta J/\delta V_k$ analytically or with the finite-difference method using Eq. (8).

We begin by optimizing the SWAP gate across multiple gate durations, ranging from 0.03 to 0.09 ms, with each time step $\Delta t = 0.005$ ms. For a simple optimization example, we use a linearly decreasing V_s as an initial guess for the pulse sequence while keeping $V_\ell = 30E_{rs}$ constant. The bounds for V_s are fixed between $2E_{rs}$ and $30E_{rs}$. The scattering length a is set to zero for the SWAP gate. The numerical optimization imposes constraints on the start and the end of the pulses to ensure that they are experimentally feasible. These constraints, in turn, force the resulting hopping parameter $J_{\text{numerical}}$ to start and end at zero. Figure 5(a) illustrates the optimized SWAP-gate error as a function of the gate duration. The infidelity decreases rapidly, becoming less than 10^{-8} for durations longer than 0.06 ms, which is close to the analytical quantum speed limit of 0.046 ms, calculated in Appendix A; however, these additional constraints prevent the optimization from fully achieving the analytical quantum speed limit. Now, as explained in Sec. II B, for the two-band Fermi-Hubbard model, basis states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ do not change under SWAP, and from the symmetry of the Hamiltonian in Eq. (11), we must reach the state $|\uparrow\downarrow\rangle$ from the initial state $|\downarrow\uparrow\rangle$. We verify this explicitly by calculating the full SWAP-gate error as

$$C_{\text{SWAP}}^F = 1 - \frac{1}{N_i} \sum_{(\Psi_{\text{ini}}, \Psi_{\text{tar}})} |\langle \Psi_{\text{tar}} | \mathcal{U}_{N_T} \cdots \mathcal{U}_1 | \Psi_{\text{ini}} \rangle|^2, \quad (16)$$

where $(\Psi_{\text{ini}}, \Psi_{\text{tar}})$ denotes the N_i different possible tuples of initial and target states. For the SWAP gate with the two-band Fermi Hubbard model, we take two sets $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ and $\{|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle\}$ and calculate the full SWAP-gate error. We show that the full SWAP-gate error exactly matches the error of transferring the state from $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$. The evolution of the three basis states is depicted in Fig. 5(b). Starting from $|\uparrow\downarrow\rangle$, the system evolves into $|\downarrow\uparrow\rangle$, while the probability of the third state $(|D0\rangle + |0D\rangle)/\sqrt{2}$ peaks at half of the gate duration. The symmetry in the time evolution also suggests that the same pulse will transfer the state $|\downarrow\uparrow\rangle$ to $|\uparrow\downarrow\rangle$. The optimized pulses V_s and V_ℓ for the 0.06-ms gate duration are shown in Fig. 5(c), where V_s approaches the minimum bound of $2E_{rs}$. Aside from the additional imposed bounds, $J_{\text{numerical}}$ attempts to reach the maximum $J = 34.03$ kHz and closely resembles $J_{\text{analytical}}$, as shown in Fig. 5(d).

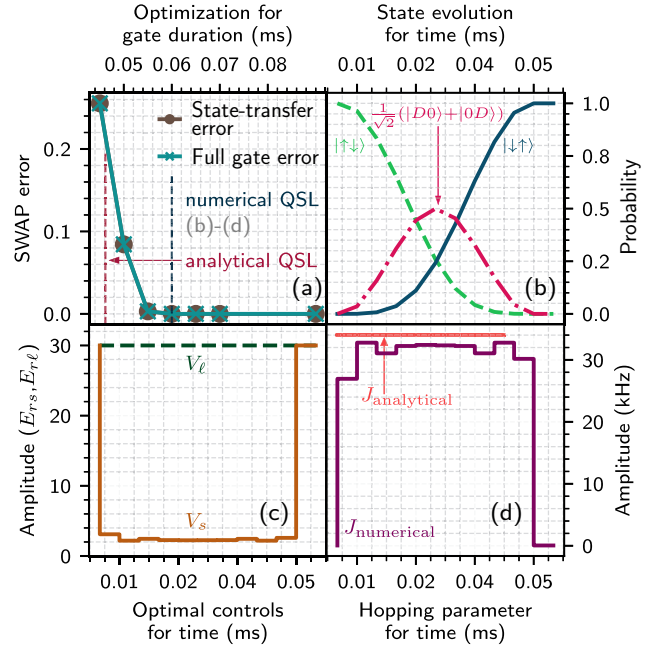


FIG. 5. (a) The error of the SWAP gate is numerically minimized for different gate durations based on a Fermi-Hubbard model; the numerical quantum speed limit (QSL) of 0.06 ms is close to the analytical one from Sec. III A, which is 0.046 ms. The full gate error defined by Eq. (16) matches the state-transfer error defined by Eq. (13). (b) Corresponding state evolution of duration 0.06 ms from $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$ with an intermediate state $(|D0\rangle + |0D\rangle)/\sqrt{2}$. The symmetry in the Hamiltonian of Eq. (11) also suggests that the same pulse will transfer the state $|\downarrow\uparrow\rangle$ to $|\uparrow\downarrow\rangle$. (c),(d) Time dependence of the optimized lattice parameters V_s and V_ℓ and hopping parameter $J_{\text{numerical}}$; a minimum V_s results in a maximal $J_{\text{numerical}}$ having a similar form as $J_{\text{analytical}}$. The discrepancy between $J_{\text{numerical}}$ and $J_{\text{analytical}}$ results from the constraints included in the optimization.

Result 2. The shortest, numerically optimized SWAP gate has a duration of 0.06 ms with an upper bound of $J_{\text{max}} = 34.03$ kHz. The corresponding pulse resembles the analytical time-optimal pulse except for the additional constraints imposed in the numerical calculations, which force $J_{\text{numerical}}$ to start and end at zero.

IV. EFFECT OF HIGHER BANDS AND OFFSITE TERMS

A. Hamiltonian description

As discussed in the previous section, atoms in the double well are described by the two-band Fermi-Hubbard model and characterized by the nearest-neighbor hopping J and the onsite interaction U ; however, if the pulses are changed nonadiabatically, the atoms may be excited within the lattice, causing the two-band Fermi-Hubbard model to fail in accurately describing the system. In such cases, it is necessary to account for the higher bands of the Fermi-Hubbard model and the offsite interactions between atoms

located on different sites in the double well. To incorporate these higher bands and offsite interactions, we generalize the two-band Hamiltonian as shown in Fig. 2. The bands appear in pairs, with each pair corresponding to one level p of the Fermi-Hubbard model, so we have $M = b/2$ levels for b bands. For instance, four bands form two levels with $p \in \{0, 1\}$, where the zeroth ($b = 0$) band and the first ($b = 1$) band form the level $p = 0$, and the second ($b = 2$) band and the third ($b = 3$) band form the level $p = 1$.

The extended higher-band Fermi-Hubbard Hamiltonian for a double well is given by

$$\hat{H} = - \sum_p \sum_{\sigma} J_p (c_{pL\sigma}^{\dagger} c_{pR\sigma} + \text{H.c.}) \quad (17a)$$

$$+ \sum_{m,n,o,p} \sum_{\alpha,\beta,\gamma,\delta} U_{mnop}^{\alpha\beta\gamma\delta} c_{m\alpha\uparrow}^{\dagger} c_{n\beta\downarrow}^{\dagger} c_{o\gamma\downarrow} c_{p\delta\uparrow} \quad (17b)$$

$$+ \sum_p \sum_{\alpha} \sum_{\sigma} \epsilon_{p\alpha} n_{p\alpha\sigma}, \quad (17c)$$

where $\alpha, \beta, \gamma, \delta \in \{L, R\}$, $m, n, o, p \in \{1, \dots, M\}$, and $\sigma \in \{\uparrow, \downarrow\}$. The term in Eq. (17a) describes hopping with amplitudes J_p for different levels p of the well, as illustrated in Fig. 6(a). Specifically, J_0 corresponds to the hopping term J in the two-band model. The hopping amplitude J_p is given by

$$J_p = - \int w_{pL}(x) \left[-\frac{\hbar^2}{2m} \partial_x^2 + V(x) \right] w_{pR}(x) dx. \quad (18)$$

The interaction strength $U_{mnop}^{\alpha\beta\gamma\delta}$ is calculated using the Wannier functions as follows:

$$U_{mnop}^{\alpha\beta\gamma\delta} = \iint U_{3D} w_{m\alpha}^{\dagger}(\mathbf{r}_1) w_{n\beta}^{\dagger}(\mathbf{r}_2) w_{o\gamma}(\mathbf{r}_2) w_{p\delta}(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2, \quad (19)$$

where $U_{3D} := U_{3D}(\mathbf{r}_1, \mathbf{r}_2)$. Finally, the Hamiltonian includes an onsite energy term corresponding to the energies ϵ_{pj} in Eq. (17c), which are calculated from

$$\epsilon_{p\alpha} = \int w_{p\alpha}(x) \left[-\frac{\hbar^2}{2m} \partial_x^2 + V(x, t) \right] w_{p\alpha}(x) dx. \quad (20)$$

While the Wannier functions associated with different bands are orthonormal, resulting in zero overlap, the integral over four different Wannier functions used in Eq. (19) is not necessarily zero; however, the interaction strength $U_{mnop}^{\alpha\beta\gamma\delta}$, which is determined by the Wannier functions, is typically negligible when $m \neq n \neq o \neq p$. Thus, we consider only the following interaction terms from Eq. (17b)

Higher-band Fermi-Hubbard model parameters

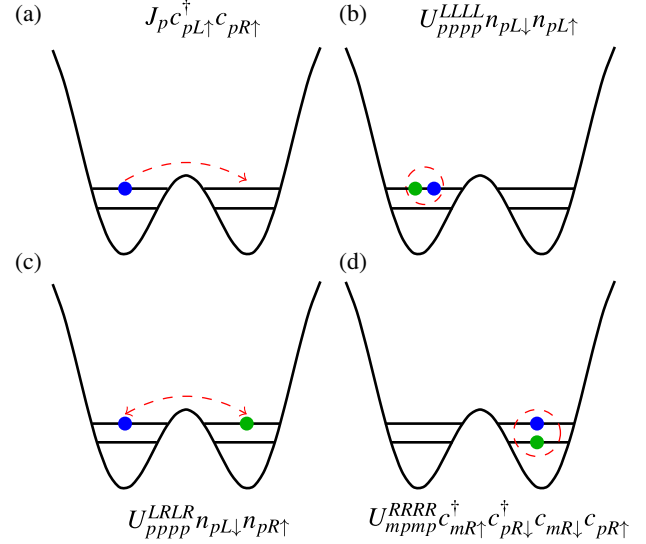


FIG. 6. Different hopping and interaction processes in a symmetric double well for a Fermi-Hubbard model with higher bands. Each level p in the double well is made from two energy bands, as shown in Fig. 2. (a) Single-atom hopping term [see Eq. (17a)] between wells for level p with hopping strength J_p calculated from Eq. (18). (b)–(d) Two atoms of opposite spin interact with strength $U_{mnop}^{\alpha\beta\gamma\delta}$ calculated from Eq. (19), where α, β, γ , and δ refer to the left (L) or the right (R) well, and m, n, o , and p denote different levels: (b) U_{pppp}^{LLLL} has two atoms on level p in the left (L) well [see Eq. (21a)]; (c) U_{pppp}^{LRLR} has two atoms on level p in different wells [see Eq. (21b)]; (d) U_{mpmp}^{RRRR} has two atoms on different levels p and m but in the right (R) well [see Eq. (21c)].

with significant contributions:

$$\hat{H}_{\text{int}} = \sum_p \sum_{\alpha} U_{pppp}^{\alpha\alpha\alpha\alpha} n_{p\alpha\downarrow} n_{p\alpha\uparrow} \quad (21a)$$

$$+ \sum_{p,m} \sum_{\alpha,\beta} \sum_{\sigma} U_{mpmp}^{\beta\alpha\alpha\beta} n_{p\alpha\sigma} n_{m\beta(-\sigma)} \quad (21b)$$

$$+ \sum_{p,m} \sum_{\alpha,\beta} U_{mpmp}^{\beta\alpha\alpha\beta} c_{m\beta\uparrow}^{\dagger} c_{p\alpha\downarrow}^{\dagger} c_{m\beta\downarrow} c_{p\alpha\uparrow} \quad (21c)$$

$$+ \sum_{p,m} \sum_{\alpha,\beta} U_{ppmm}^{\alpha\alpha\beta\beta} c_{p\alpha\uparrow}^{\dagger} c_{p\alpha\downarrow}^{\dagger} c_{m\beta\downarrow} c_{m\beta\uparrow} \quad (21d)$$

$$+ \sum_p \sum_{\alpha} \sum_{\sigma} U_{pppp}^{\alpha\alpha LR} n_{p\alpha,-\sigma} (c_{pL\sigma}^{\dagger} c_{pR\sigma} + \text{H.c.}). \quad (21e)$$

Remark 3. For Eqs. (21b)–(21d), we only consider interaction terms such that the two atoms either have the same energy levels p and m or they sit on the same side α and β of the double well, i.e.,

$$p = m \text{ if } \alpha \neq \beta \quad \text{and} \quad \alpha = \beta \text{ if } p \neq m.$$

The interaction term in Eq. (21a) involves onsite interactions with strengths $U_{pppp}^{\alpha\alpha\alpha\alpha}$, corresponding to interactions at level p and on side α , as shown in Fig. 6(b). Additionally, during gate operations, the short-lattice depth V_s decreases significantly, as depicted in Fig. 5(c). Consequently, the barrier between the double well becomes sufficiently small that atoms on either side or at different levels start to interact. This is represented by the offsite interaction term $n_{p\alpha\sigma} n_{m\beta(-\sigma)}$, which is proportional to $U_{mppm}^{\beta\alpha\alpha\beta}$, as described in Eq. (21b) and illustrated in Fig. 6(c). The term $c_{m\beta\uparrow}^\dagger c_{p\alpha\downarrow}^\dagger c_{m\beta\downarrow} c_{p\alpha\uparrow}$ in Eq. (21c) and Fig. 6(d) describes the spin-exchange process with strength $U_{mmpm}^{\beta\alpha\alpha\beta}$ between two atoms at levels p and m and on sides α and β . The term $c_{p\alpha\uparrow}^\dagger c_{p\alpha\downarrow}^\dagger c_{m\beta\downarrow} c_{m\beta\uparrow}$ in Eq. (21d) represents the correlated pair tunneling of two atoms within the double well.

Lastly, we have a correction term proportional to $\Delta J_{p\alpha} = U_{pppp}^{\alpha\alpha LR}$ in Eq. (21e), which yields

$$\Delta J_{p\alpha} = \iint U_{3D} |w_{p\alpha}(\mathbf{r}_1)|^2 w_{pL}(\mathbf{r}_2) w_{pR}(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2. \quad (22)$$

This term accounts for density-assisted hopping, which corrects the hopping parameter J_p when another atom of opposite spin is in the double well on side α .

B. Simulations

To study the effects of these new terms, we perform a time evolution of the system using the Hamiltonian in Eq. (17) with a nonadiabatic approach. Because the x -direction terms of the potential in Eq. (1) change nonadiabatically while keeping the y - and z -direction terms constant, the Wannier functions in the x -direction vary at each time step during the evolution. Consequently, after each unitary evolution at time step t , we compute the updated Wannier functions w_t and transform the evolved state onto these new Wannier states. The nonadiabatic time evolution is described by

$$\Psi(t+1) = P(w_{t+1}, w_t) e^{-iH_t \delta t} \Psi(t). \quad (23)$$

Here, $P(w_{t+1}, w_t)$ denotes the basis-transformation operator, which describes the nonadiabaticity of the time evolution by changing the basis of the state into the new Wannier basis states at every time step. Since calculating the Wannier functions as described in Sec. II is necessary to construct $P(w_{t+1}, w_t)$ for each time step, we cannot use the spline method employed in Sec. III B; instead, we must directly compute the parameters J , U , ΔJ , and ϵ from Eqs. (18)–(20) for each time step.

We use this simulation method to assess the validity of the two-band model. We simulate the four- and six-band Fermi-Hubbard models using the pulses optimized from the two-band model. We optimize the SWAP gate for various durations ranging from 0.05 to 0.35 ms within the two-band Fermi-Hubbard model [see Sec. III B]. Figure 7(a)

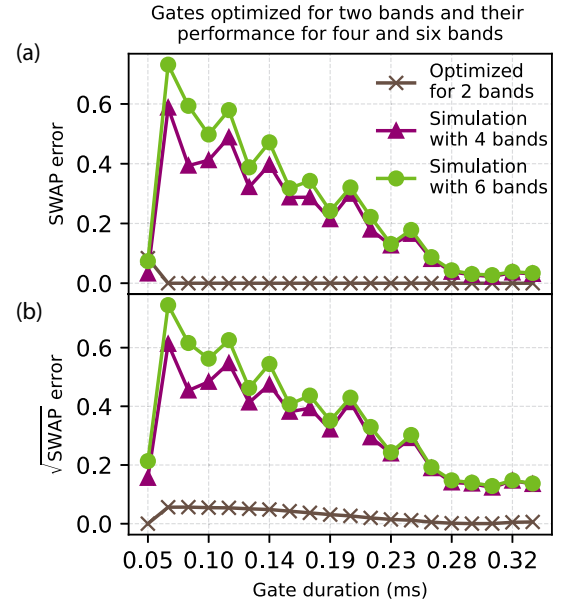


FIG. 7. The SWAP and $\sqrt{\text{SWAP}}$ gates have been numerically optimized using a two-band Fermi-Hubbard model for different gate durations as in Fig. 5(a). Their performance is compared to Fermi-Hubbard simulations with four and six bands. (a) For SWAP, we see much higher gate errors for four and six bands than for two bands for gate durations of less than 0.28 ms, while (b) high gate errors are observed for $\sqrt{\text{SWAP}}$ with four and six bands and all gate durations.

presents the infidelities for the two-band model at different gate durations. It is evident that high-fidelity gates can be achieved for very short gate durations using the two-band model. We then apply these optimized control pulses to simulate the four- and six-band models. As shown in Fig. 7(a), the simulations with higher bands exhibit significant deviations from the two-band results, with the discrepancies increasing for shorter gate durations.

We conduct a similar analysis for the $\sqrt{\text{SWAP}}$ gate, as shown in Fig. 7(b). Here, we use the optimized time-dependent lattice depths V_s and V_ℓ from the SWAP-gate optimizations and optimize only the time-independent scattering length a using the two-band model. The interaction strength U is calculated from a using Eq. (9). Figure 7(b) shows that, similar to the SWAP gate, very low infidelities for the $\sqrt{\text{SWAP}}$ gate can be achieved using the two-band Fermi-Hubbard model. Next, we simulate the four- and six-band models using the optimal controls from the two-band model. For short gate durations, we again observe significant divergence of the higher-band simulations from the two-band model results [see Fig. 7(b)]; however, unlike the SWAP gate, the higher-band simulations fail to match the two-band results even for longer gate durations in the case of the $\sqrt{\text{SWAP}}$ gate. This discrepancy is likely due to the additional offsite interactions present in the higher-band model [see Eq. (17)], whereas

the two-band model includes only onsite interactions. Furthermore, in the two-band model, the Wannier states used in Eq. (9) are computed at the start of the time evolution and are assumed to remain constant throughout. This assumption holds for an adiabatic time evolution, where the initially calculated Wannier states are eigenstates of the Hamiltonian at all times; however, for fast gates with nonadiabatic changes in lattice depths, the Wannier states $w_{pL}(t)$ and $w_{pR}(t)$ vary during the evolution. This variation introduces additional errors in the gate fidelity, which are accounted for in the higher-band simulations through the basis-transformation operators in Eq. (23).

Result 3. Simulations in higher-band Fermi-Hubbard models of pulses optimized using a two-band model show significantly higher errors for the SWAP and $\sqrt{\text{SWAP}}$ gates. This suggests that for nonadiabatic gate operations, the two-band model is not sufficient, and optimizations using higher-band Fermi-Hubbard models are essential.

V. OPTIMIZATION WITH HIGHER-BAND FERMİ-HUBBARD MODEL

We showed in Sec. IV that optimization with a two-band Fermi-Hubbard model is insufficient for describing fast SWAP and $\sqrt{\text{SWAP}}$ gates. To better capture the behavior of the system and generate efficient gates, we must include higher bands of the model in our optimization. In analogy to the two-band model, we optimize the SWAP and $\sqrt{\text{SWAP}}$ gates using gradient-based methods with a higher-band Fermi-Hubbard model. We use the nonadiabatic simulation method described in Sec. IV B. We optimize V_s and V_ℓ for the SWAP gate with the scattering length $a = 0$. In contrast to the two-band model, where the $\sqrt{\text{SWAP}}$ gate is controlled by the lattice depths V_s and V_ℓ from the SWAP-gate optimization, we independently optimize V_s and V_ℓ for the target state $\Psi_{\sqrt{\text{SWAP}}}$ and then perform

ALGORITHM 2. Optimization of the SWAP and $\sqrt{\text{SWAP}}$ gates with higher-band models

SWAP: Same as in the SWAP optimization in Algorithm 1. Instead of the spline-fit method, a combination of approximate analytical and finite-difference gradients is used.

$\sqrt{\text{SWAP}}$:

Optimization parameters: $V_s(t)$, $V_\ell(t)$, and a

Step 1: Define the $\sqrt{\text{SWAP}}$ -gate cost function $C_{\sqrt{\text{SWAP}}} = 1 - |\langle \Psi_{\sqrt{\text{SWAP}}} | \Psi(T) \rangle|^2$

Step 2: Minimize $C_{\sqrt{\text{SWAP}}}$ and optimize $V_s(t)$ and $V_\ell(t)$ using a gradient-based optimization

Step 3: Perform a one-dimensional search to find the optimized a for $C_{\sqrt{\text{SWAP}}}$

Output: Optimized $V_s(t)$, $V_\ell(t)$, and a for $\sqrt{\text{SWAP}}$

a one-dimensional search to find the optimal a . This is described in Algorithm 2. For the two-band model in Sec. III B, we calculate the gradient of the cost function C with respect to V_s and V_ℓ using a spline-fit method, whereas the gradient for the one-dimensional search is trivial and easily computed using finite differences. Nonetheless, for the higher-band model, in the absence of a spline-fitting approach, the gradients dC/dV_s and dC/dV_ℓ can be computed either analytically or through finite differences. In Appendix B, we derive an approximate analytical expression for the gradient that is considerably faster than the finite-difference method, as shown in Appendix C. This approximation allows for an accelerated optimization process. Subsequently, we can employ the finite-difference method to refine the optimization, enabling convergence to the minimum of the cost function.

A. State-to-state transfer optimization

First, we optimize the transfer from the initial state Ψ_0 to the target state Ψ_{SWAP} , for different gate durations using the four-band Fermi-Hubbard model. We try to find the optimal V_s and V_ℓ for variable gate durations from 0.06 to 0.20 ms. We constrain the optimization with bounds on V_s and V_ℓ given by the pairs $(0.1 E_{rs}, 45 E_{rs})$ and $(7 E_{r\ell}, 35 E_{r\ell})$, respectively. The optimized SWAP infidelities are presented in Fig. 8(a), where the error is less than 0.001 for gate durations longer than 0.08 ms. We emphasize that compared to the four-band simulation in Fig. 7(a), we achieve a significantly lower infidelity after optimizing for the four-band model with similar gate durations. The improvement in fidelity comes from the enhanced controllability by including the higher bands with multiple hopping parameters. To validate the four-band model, we simulate the system with six bands using the optimized controls from the four-band optimization. The gate error in the six-band model shows negligible deviation from the error in the four-band model [see Fig. 8(a)]. Specifically, the error in the six-band simulation is less than 0.001 for gate durations greater than 0.1 ms. This result suggests that excitations beyond four bands are negligible, indicating that the four-band Fermi-Hubbard model is sufficient to capture most of the dynamics of the double-well system under the SWAP gate. We also examine the effect of the upper bound of the long-lattice depth V_ℓ on the gate fidelity. The SWAP gate is optimized for upper bounds given by 30, 40, and 50 times the value of $E_{r\ell}$, and the resulting infidelities are shown in Fig. 8(b) on a logarithmic scale. We observe that the gate fidelity improves with a higher upper bound on V_ℓ , as an increased V_ℓ leads to more localized Wannier states and enhances the hopping strength J .

Next, we optimize the lattice depths V_s and V_ℓ and the scattering length a for the $\sqrt{\text{SWAP}}$ gate, i.e., for transferring the state Ψ_0 to the state $\Psi_{\sqrt{\text{SWAP}}}$, using the same initial conditions and bounds as in the SWAP-gate optimization.

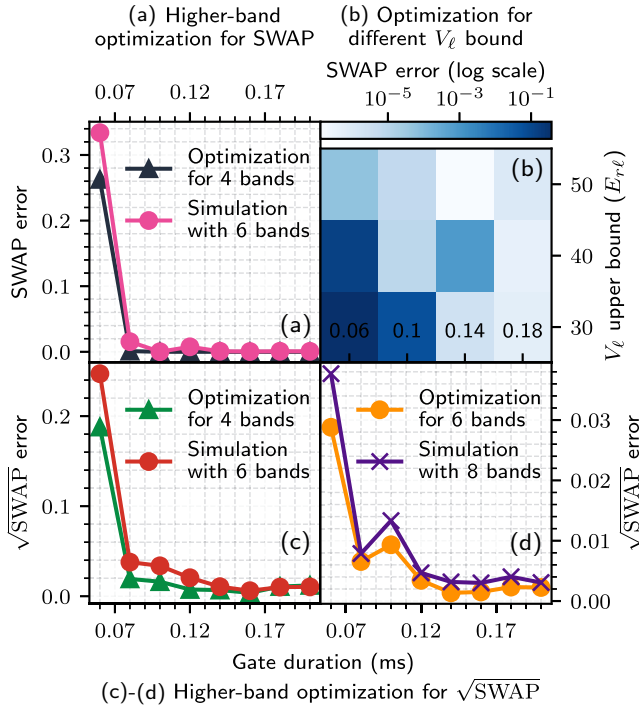


FIG. 8. Higher-band Fermi-Hubbard optimizations for SWAP and $\sqrt{\text{SWAP}}$. (a) The SWAP-gate optimizations for four bands have an error of less than 0.001 for gate durations of more than 0.08 ms. These optimized pulses for four bands are used in six-band simulations, whose results closely match, with errors of less than 0.001 for gate durations greater than 0.1 ms. This suggests that four-band optimizations are sufficient for the high-fidelity SWAP gate. (b) SWAP-gate optimization errors for upper bounds given by 30, 40, and 50 $E_{r\ell}$ for V_ℓ and the four-band model; For each upper bound, the error is shown with gate durations of 0.06, 0.1, 0.14, and 0.18 ms. Larger upper bounds result in smaller gate errors, especially for shorter gate durations. (c) Similar optimizations and simulations for $\sqrt{\text{SWAP}}$. The four-band optimizations have errors of less than 0.007 for gate durations greater than 0.12 ms. The corresponding six-band simulations slightly differ, with errors of less than 0.007 for gate durations greater than 0.16 ms. (d) Improved $\sqrt{\text{SWAP}}$ optimizations with errors of less than 0.005 for gate durations greater than 0.12 ms achieved by increasing the upper bound for V_ℓ to 45 $E_{r\ell}$ and optimizing for six bands. The corresponding eight-band simulations have errors of less than 0.005 for gate durations greater than 0.12 ms and show negligible excitation beyond six bands.

As shown in Fig. 8(c), the infidelity increases for shorter pulse durations. The four-band optimizations yield errors of less than 0.007 for gate durations longer than 0.12 ms. Similar to the SWAP gate, we compare our results with six-band simulations, as illustrated in Fig. 8(c). The six-band simulations differ slightly from the four-band results, showing errors of less than 0.007 for gate durations longer than 0.16 ms, indicating the presence of higher-band excitations in the system. This can be mitigated by increasing the upper bound on V_ℓ to 45 $E_{r\ell}$ and optimizing within the

six-band model, as shown in Fig. 8(d). We further compare the optimization in the six-band model with simulations in the eight-band model and observe negligible excitations beyond six bands. Both the six-band optimization and the eight-band simulation result in gate errors smaller than 0.005 for gate durations longer than 0.12 ms. This suggests that for the $\sqrt{\text{SWAP}}$ gate, good pulses can be identified through four- or six-band optimizations, with the six-band model producing lower higher-band excitation compared to the four-band model.

B. Dynamics with optimized controls

We focus on one set of optimal lattice depths V_s and V_ℓ for a duration of 0.12 ms, as shown in Fig. 9(a), which have been optimized for the $\sqrt{\text{SWAP}}$ gate. The optimal scattering length is $a = 1995.22a_0$, where $a_0 = 5.29 \times 10^{-11}$ m is the Bohr radius. The controls are simple and realistic, adhering to experimental constraints. The corresponding time evolutions for the SWAP and $\sqrt{\text{SWAP}}$ gates are illustrated in Figs. 9(b) and 9(c), respectively. The system begins in the state Ψ_0 and evolves to the target states Ψ_{SWAP} and $\Psi_{\sqrt{\text{SWAP}}}$ for the SWAP and $\sqrt{\text{SWAP}}$ gates, respectively. The symmetry in the system suggests that the same pulse will transfer the state Ψ_{SWAP} to Ψ_0 for the SWAP gate. Notably, there is excitation and de-excitation from higher-band states during the time evolution, resulting in faster gate operations. The combined probabilities for all the states involving the second level are less than 10^{-7} and 10^{-4} at the end of the SWAP and $\sqrt{\text{SWAP}}$ gates, respectively. This suggests that the optimized controls effectively minimize excitations to higher levels at the end of the gates, which is crucial for any quantum operation. The remaining error arises from probabilities of the order of 10^{-3} for the first-level states $|D0\rangle$ and $|0D\rangle$ in the case of the $\sqrt{\text{SWAP}}$ gate.

We also examine the impact of the optimal V_s , V_ℓ , and a on the higher-band Fermi-Hubbard parameters of Eq. (17). Each level p in the double well is composed of two energy bands, $2p$ and $2p + 1$, yielding two levels in the four-band Fermi-Hubbard model. The hopping parameter J_0 represents the hopping between the left (L) and right (R) sides of the well on the first level (or equivalently the hopping J of the two-band Fermi-Hubbard model), and $U_{0000}^{\alpha\alpha\alpha\alpha}$ corresponds to the interaction U of the two-band Fermi-Hubbard model, as shown in Fig. 9(d). The value of J_0 increases with decreasing V_s and increasing V_ℓ , as these conditions lead to a higher overlap between the Wannier functions w_{0L} and w_{0R} . Conversely, the onsite interaction $U_{0000}^{\alpha\alpha\alpha\alpha}$ decreases with decreasing V_s , as shown in Fig. 9(d).

For the two-band Fermi-Hubbard model optimization in Sec. III B, we assume that the interaction strength is independent of changes in the Wannier functions and remains constant and proportional to a ; however, we observe that this assumption breaks down with our optimal

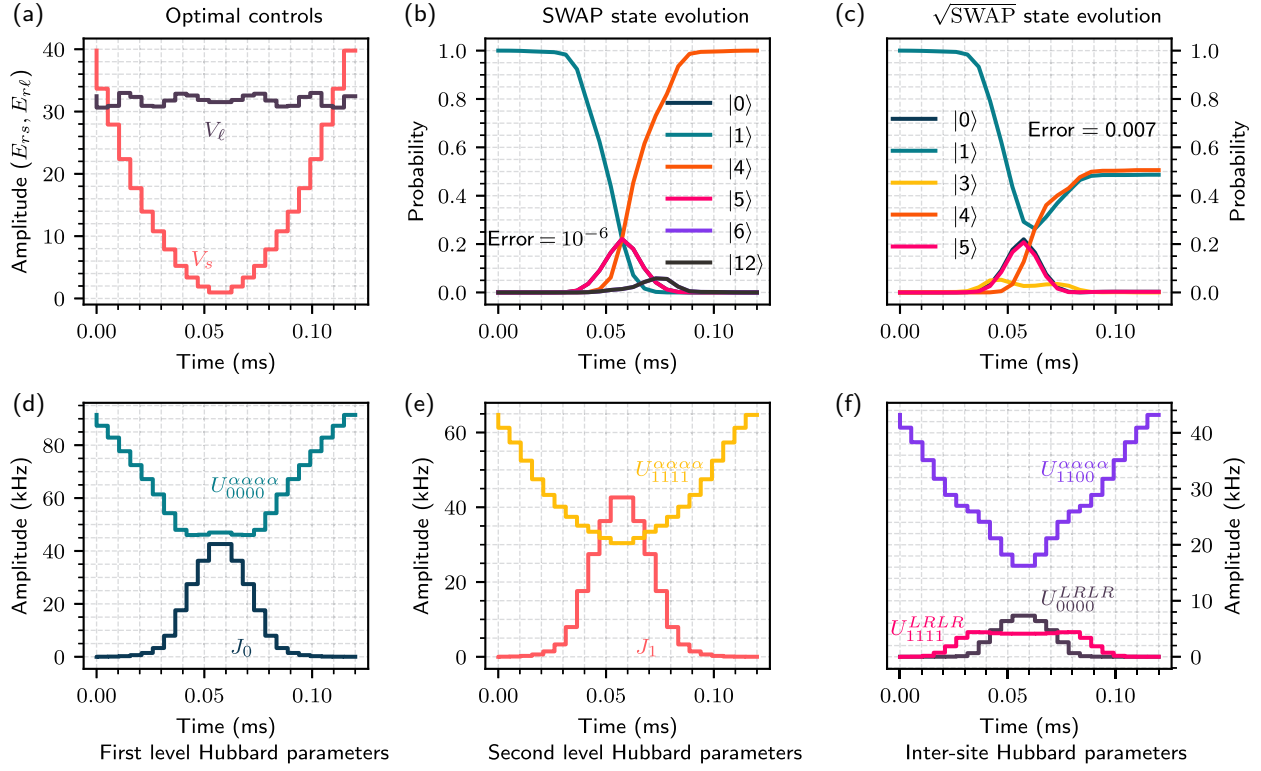


FIG. 9. Four-band Fermi-Hubbard-model optimizations for a short gate duration of 0.12 ms relying on excitations to higher bands and multiple hopping and interaction strengths. (a) Optimal controls V_s and V_ℓ in their respective recoil energies $E_{rs(\ell)} = \hbar^2 k_{s(\ell)}^2 / (2m)$. (b) State evolution under SWAP from $|1\rangle = |\uparrow\downarrow\rangle$ to $|4\rangle = |\downarrow\uparrow\rangle$ for 0.12 ms with optimal controls from (a) and the state-labeling scheme in Sec. VI and Table. II. (c) State evolution under $\sqrt{\text{SWAP}}$ from $|1\rangle = |\uparrow\downarrow\rangle$ to $[(1+i)|1\rangle - (1-i)|4\rangle]/2 = [(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$ with optimal controls from (a) and optimized scattering length $a = 1995.22 \times a_0$, where $a_0 = 5.29 \times 10^{-11}$ m is the Bohr radius. (d)–(f) Corresponding Fermi-Hubbard parameters: Each level p in the double well consists of two energy bands $2p$ and $2p + 1$, resulting in two levels for the four-band Fermi-Hubbard model. (d) The hopping parameter J_0 on the first level and between the left and right sides of the double well increases with decreasing V_s and increasing V_ℓ . The onsite interaction $U_{0000}^{\alpha\alpha\alpha\alpha}$ on the first level is directly proportional to V_s and V_ℓ . (e) The second-level hopping parameter J_1 and the onsite interaction $U_{1111}^{\alpha\alpha\alpha\alpha}$ behave similarly to those in (d). (f) The offsite interaction U_{0000}^{LRLR} and U_{1111}^{LRLR} between the left and right sides on the first and second levels have small magnitude and become significant for small V_s . Here, $U_{1100}^{\alpha\alpha\alpha\alpha}$ represents the interaction between the first and second levels on the same side of the double well and behaves similarly to $U_{pppp}^{\alpha\alpha\alpha\alpha}$.

lattice depths for the four-band Fermi-Hubbard model, as V_s becomes shallow for fast gates. In the four-band Fermi-Hubbard model, an additional hopping parameter J_1 and onsite interaction strength $U_{1111}^{\alpha\alpha\alpha\alpha}$ arise, as shown in Fig. 9(e). The parameter J_1 has a larger magnitude compared to J_0 because the overlap between the Wannier functions w_{1L} and w_{1R} for the second level is greater than that for the first level. Conversely, $U_{1111}^{\alpha\alpha\alpha\alpha}$ has a smaller magnitude compared to $U_{0000}^{\alpha\alpha\alpha\alpha}$ due to the reduced overlap of the Wannier functions on the same site at the second level. Additionally, there are significant contributions from offsite interactions $U_{mnop}^{\alpha\beta\gamma\delta}$ when the lattice depths are shallow.

Figure 9(f) illustrates the variation of three different offsite interactions with time-dependent lattice depths. The terms U_{0000}^{LRLR} and U_{1111}^{LRLR} represent the offsite interactions between the left (L) and right (R) sides of the double well

for the first and second levels, respectively. Similar to J_p , the offsite interaction U_{pppp}^{LRLR} is proportional to the overlap between the wave functions on the left and right sides; thus, it increases as V_s decreases. The term $U_{1100}^{\alpha\alpha\alpha\alpha}$ represents the interaction between atoms occupying different levels but residing on the same side α . For $U_{pppp}^{\alpha\alpha\alpha\alpha}$, the interaction $U_{1100}^{\alpha\alpha\alpha\alpha}$ decreases as the Wannier functions spread out with a shallower short lattice.

Note that the optimized gates are distinct from superexchange processes where $U \gg J$, which avoid the $|D0\rangle$ and $|0D\rangle$ states but result in long gate times [36]. For the optimized pulses shown in Fig. 9(a), we obtain $U_{0000}^{\alpha\alpha\alpha\alpha}/J_0 = 5.34$ and $U_{1111}^{\alpha\alpha\alpha\alpha}/J_1 = 3.64$, where these ratios are calculated by integrating the time-dependent curves in Figs. 9(d) and 9(e). This ratio is close to the exchange ratio $U/J = 4/\sqrt{3}$, which permits population in the $|D0\rangle$ and $|0D\rangle$ states. Our optimized control operates near this exchange

ratio but is further refined to minimize population in the $|D0\rangle$ and $|0D\rangle$ states while achieving faster gates. Similar parameter regimes could be accessed through adiabatic control, but this would result in slower gates. The speedup in our case arises from nonadiabatically modulating V_s and V_ℓ to dynamically enhance J from an initially negligible value. This results in pulses that are experimentally feasible and helps efficiently manage excitations to higher energy levels.

Result 4. Efficient SWAP and $\sqrt{\text{SWAP}}$ gates are found using higher-band Fermi-Hubbard models. The control duration can be as short as 0.08 ms for transferring the state Ψ_0 to Ψ_{SWAP} and 0.12 ms for transferring Ψ_0 to $\Psi_{\sqrt{\text{SWAP}}}$, which is five times shorter than typical experimental state-transfer durations [44,45]. The results for $\sqrt{\text{SWAP}}$ are improved by optimizing with the six-band model and increasing the upper bound on V_ℓ .

In Secs. VI and VII, we discuss how the obtained gates perform when they are applied to error states with three and four atoms in a double well, as well as their robustness under multiple error sources. After this, we consider the full gate optimization using higher bands in the Fermi-Hubbard model (see Sec. VIII).

VI. MULTI-ATOM DYNAMICS

We have demonstrated performance enhancements for SWAP and $\sqrt{\text{SWAP}}$ for two atoms of opposite spins in a double well; however, in a real experimental setup, multiple double wells are controlled by global lasers V_s and V_ℓ , and some double wells may contain more or fewer than two atoms after state preparation. To fully characterize the system, it is essential to consider all possible atomic configurations within a double well and analyze the impact of our optimized pulses on these configurations. For fermionic atoms, 16 different states can exist within a double well with up to four atoms:

- (a) 0 atoms: $|00\rangle$,
- (b) 1 atom: $|\uparrow 0\rangle, |0 \uparrow\rangle, |\downarrow 0\rangle, |0 \downarrow\rangle$,
- (c) 2 atoms: $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |D0\rangle, |0D\rangle$,
- (d) 3 atoms: $|D \uparrow\rangle, |\uparrow D\rangle, |D \downarrow\rangle, |\downarrow D\rangle$,
- (e) 4 atoms: $|DD\rangle$,

where $D = \uparrow\downarrow$ represents a double occupancy on one side of the double well. One-atom states serve as single-qubit states, and for two-qubit gates, states with three and four atoms are error states. For adiabatic gates, the three-atom states behave similarly to the one-atom states, and the four-atom state $|DD\rangle$ remains unchanged, as both sites are already fully occupied; however, for fast gate operations, these doubly occupied atoms can be individually excited to higher energy levels within the double well.

We investigate the dynamics of various atomic configurations in a double well using the method described in Appendix D for calculating and assigning the computational states with a given number of atoms. For this comparison, we employ the optimized controls V_s , V_ℓ , and a derived for the two-atom $\sqrt{\text{SWAP}}$ gate from Sec. V A. The optimized gate errors for the two-atom case are repeated in Fig. 10(a) for reference. In the ideal scenario, the single-atom states undergo a SWAP operation from the left to the right side of the double well, or vice versa. This implies that our initial state for the one-atom case is $I = 0$ and the target state is $I = 1$. As illustrated in Fig. 10(a), the state-evolution error of the one-atom dynamics corresponding to a state with $N_\uparrow = 1$ and $N_\downarrow = 0$ is negligible, as the single atom is unaffected by the atom-atom interaction induced by a . Similarly, in an ideal situation, the three-atom states should also perform a SWAP operation. For example, if the initial state is $|D \uparrow\rangle$, the target state should be $|\uparrow D\rangle$; however, as shown in Fig. 10(a), the error for the three-atom configurations with $N_\uparrow = 2$ and $N_\downarrow = 1$ increase with shorter pulses due to the atom-atom interactions and excitations to higher energy levels. A similar analysis was conducted for the four-atom state with $N_\uparrow = 2$ and $N_\downarrow = 2$, where both the initial and target states are the same, i.e., $|DD\rangle$. This state exhibits higher state-evolution error compared to the three-atom states, as more atoms are excited to higher levels and undergo multiple atom-atom interactions. The three- and four-atom configurations converge to infidelities below 0.1 for a gate duration of 0.20 ms.

The time evolutions for one-, two-, three-, and four-atom cases under a gate duration of 0.20 ms are presented in Figs. 10(b)–10(e), respectively. In the one-atom case, the system evolves from the state $|\uparrow 0\rangle$ to $|0 \uparrow\rangle$, demonstrating the desired dynamics, as shown in Fig. 10(b). For the two-atom case, the system performs the $\sqrt{\text{SWAP}}$ gate with high fidelity, transitioning from Ψ_0 to $\Psi_{\sqrt{\text{SWAP}}}$, as depicted in Fig. 10(c). In the three-atom case, starting from $|D \uparrow\rangle$, the system evolves to $|\uparrow D\rangle$ with an infidelity of 0.09 [see Fig. 10(d)]. Finally, the four-atom state $|DD\rangle$ is shown to excite to higher bands, resulting in an error of 0.027 in maintaining the $|DD\rangle$ state [see Fig. 10(e)]. It is important to note that in Figs. 10(b)–10(e), we only display the states that exhibit probabilities greater than 0.05 at any time step during the evolution.

Remark 4. The optimized pulses for the $\sqrt{\text{SWAP}}$ gate from Fig. 8(c) result in a high state-evolution infidelity for error states with three and four atoms compared to states with one and two atoms. In particular, for shorter pulse durations, the atoms interact with each other and excite to the higher bands; however, these error states can be suppressed with good initial state preparation, rendering them less significant for gate operations.

If necessary, the optimization protocols can be extended to include infidelities from different atomic configurations

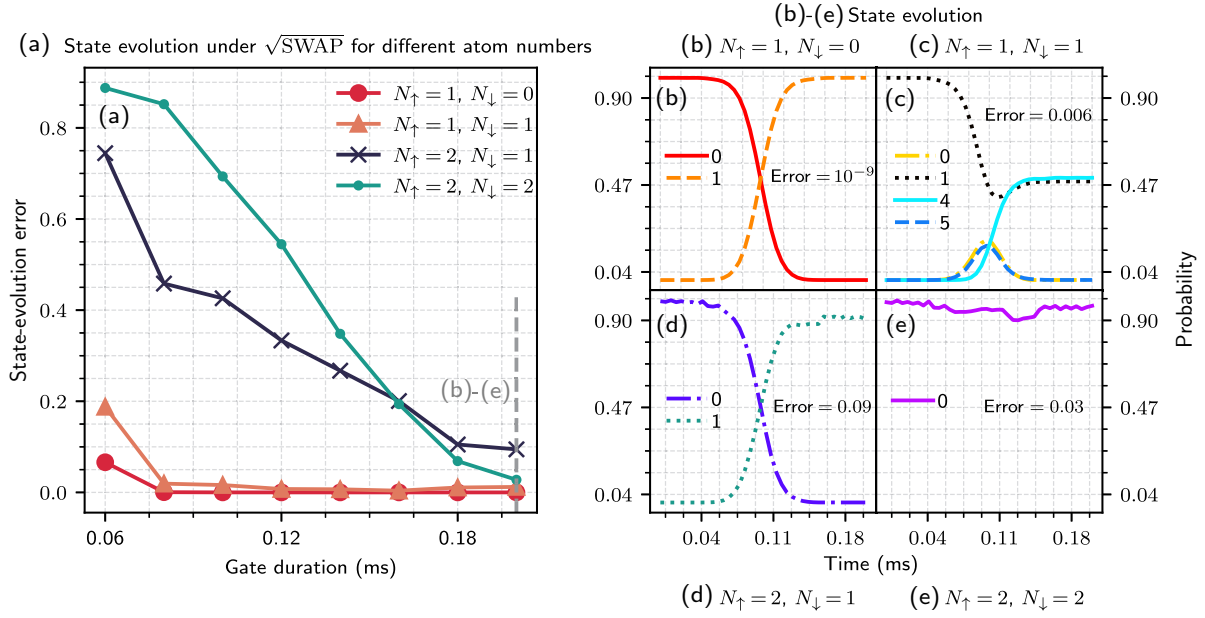


FIG. 10. State-evolution errors under $\sqrt{\text{SWAP}}$ for different numbers of atoms using the optimized control pulses from Fig. 8(c) as compared to the usual case of two atoms with $N_\uparrow = 1$ and $N_\downarrow = 1$ in a double well and measured with a four-band Fermi-Hubbard simulation. (a) Single atoms with $N_\uparrow = 1$ and $N_\downarrow = 0$ have an infidelity of less than 0.0005 for gate durations greater than 0.08 ms. Two atoms with $N_\uparrow = 1$ and $N_\downarrow = 1$ agree with the optimized infidelities from Fig. 8(c). The error states with three and four atoms with either $N_\uparrow = 2$ and $N_\downarrow = 1$ or $N_\uparrow = 2$ and $N_\downarrow = 2$ result in higher infidelities of around 10^{-2} for a duration of 0.20 ms. (b)–(e) Corresponding state evolutions for a duration of 0.20 ms. Further optimizations are possible for error states with three or four atoms if required.

in the cost function defined in Eq. (16), optimizing the full dynamics for more comprehensive experimental scenarios.

VII. ROBUSTNESS OF THE OPTIMIZED CONTROL PULSES

In this section, we assess the robustness of the optimal control pulses in the presence of different types of error sources [44,45]. The first error source involves potential tunneling from the target double well to neighboring wells. This means that during the gate operation, the atom has a finite probability of moving to the neighboring wells, which reduces the gate fidelity. To test the robustness of the optimal control pulses against interwell tunneling, we use a set of optimized V_s and V_ℓ obtained from the SWAP optimization [see Sec. V A] of 0.08-ms duration and 0.999 fidelity, as shown in Fig. 8(a). We simulate a system with three double wells, where the middle double well is our target well and the left and right double wells act as the neighboring wells. We take only half of the adjacent left and right double wells, resulting in eight possible states, with two on the left double well, four on the middle double well, and two on the right double well for a single atom within the four-band model. In Fig. 11(a), we present the time evolution of the states in the neighboring wells during the gate operation. Here, $L1$ and $L2$ represent the first and second levels of the left neighbor, while $R1$ and $R2$

are the first and second levels of the right neighbor. When the atoms are in the first level, the overlap of the Wannier functions of different double wells is low, resulting in small hopping probabilities $L1$ and $R1$. The hopping probabilities $L2$ and $R2$ increase slightly when the atoms are in the second level due to the higher overlap of the Wannier functions, as shown in Fig. 11(a). The maximum probability of the atom tunneling to states outside the target double well at any time is negligible (approximately 10^{-3}), and the atom also tunnels back to the target double well because the probabilities in the neighboring wells decrease. This analysis considers the case where the neighboring double wells are initially empty. When the neighboring wells are occupied by atoms, the hopping probabilities change accordingly. For example, if there is an atom in the neighboring well with the same spin as the hopping atom, the hopping will be suppressed due to the Pauli exclusion principle; however, if the atoms have opposite spins and the scattering length a is nonzero, the hopping will slightly increase due to a correction from the density-assisted hopping term, similar to Eq. (22).

The second error comes from the phase instability of the lattice potential. In our simulations, we consider a symmetric double well with a relative phase of $\phi = 0$, but in a real experiment, the relative phase fluctuations can lead to dephasing. Phase errors can generally be categorized into two types. The first type consists of time-independent

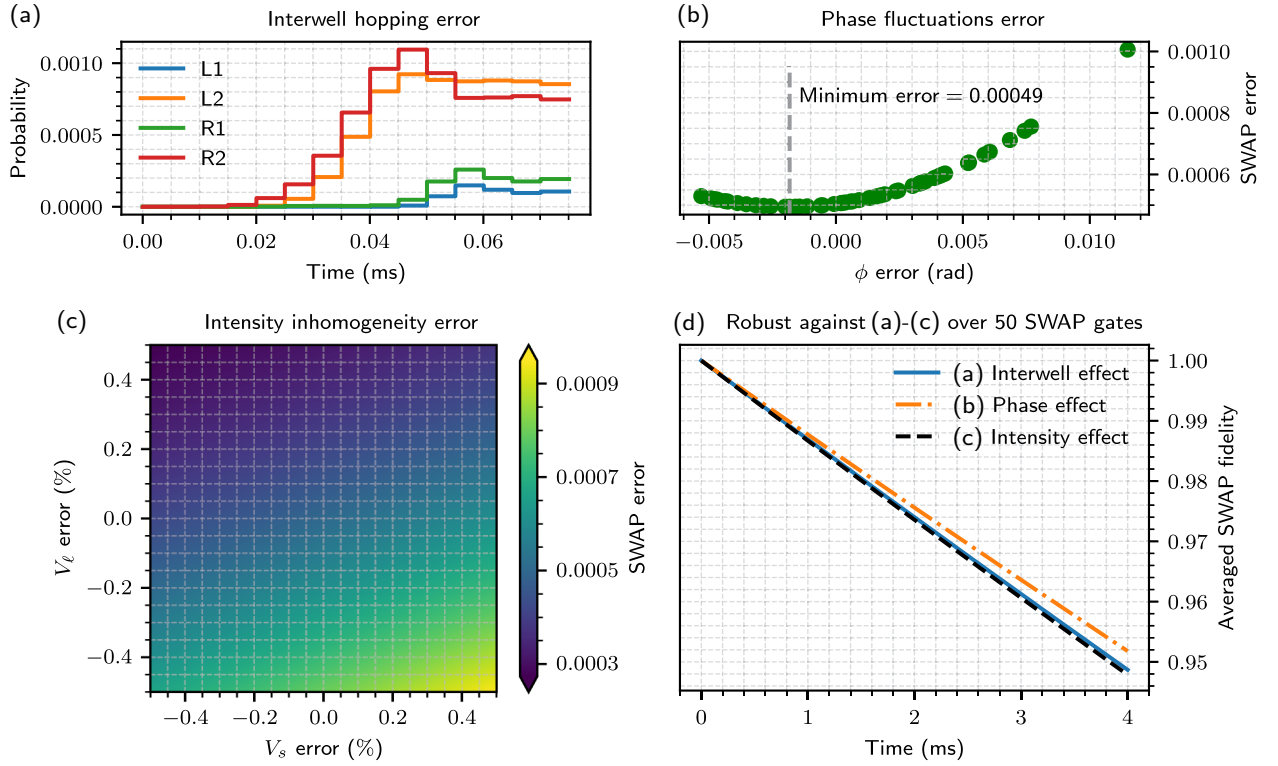


FIG. 11. Robustness of a SWAP gate against interwell hopping, phase fluctuations, and intensity inhomogeneity for an optimized control with a duration of 0.08 ms: (a) interwell hopping for three double wells, where $L1$, $L2$, $R1$, and $R2$ denote the probability of the atom being in the first and second levels of the adjoining left and right double wells, respectively. (b) Phase-fluctuation errors from numerically introduced errors in the relative phase chosen from a Gaussian distribution with a standard deviation of 4.5 mrad [44]. (c) Intensity-inhomogeneity errors from numerically introduced errors in the laser depths V_s and V_l chosen uniformly within $\pm 0.5\%$ [44]. (d) Exponential fit for the SWAP fidelity for each error source from (a)–(c) using 50 SWAP gates. The intensity inhomogeneity is the dominant source of error, whereas phase fluctuations are the smallest. For all errors, the exponential decay time of $\tau_d > 74$ ms (or 460 gates) predicts a very long coherence time for the chosen error strengths [44,45].

or static phase fluctuations, which introduce a constant energy offset in the system. The second type consists of time-dependent phase fluctuations or drifts, which, if sufficiently strong, can lead to dephasing effects. In our work, we incorporate the static phase error into Eq. (2), resulting in an energy offset between the left and right sites of the double well, thereby modifying the effective hopping amplitude. This alteration contributes to an increase in the gate error. When the gate is applied repeatedly over multiple cycles, this accumulated error leads to the damping of the Rabi oscillations, manifesting as a loss of coherence in the system's dynamics. To understand the impact of these fluctuations, we sample 50 phase errors from a Gaussian distribution with a 4.5-mrad standard deviation [44]. We simulate our four-band model using these 50 phase errors with the same controls of 0.08-ms duration. As shown in Fig. 11(b), the infidelity increases negligibly as ϕ changes, demonstrating the robustness of the controls against phase fluctuations.

Lastly, we study the effect of the inhomogeneity in the laser intensities. These inhomogeneities lead to different

coupling strengths across the lattice resulting in different gate errors. We test the robustness of the controls V_s and V_l against these fluctuations by uniformly selecting 400 pulses on a 20×20 grid with extremal values given by the pairs $(V_s \pm e, V_l \pm e)$ and an error of $e \leq 0.5\%$ [44]. Figure 11(c) shows that the infidelity increases with increasing V_s error as a result of decreasing tunneling strength J . For increasing V_l , J increases and results in a decreasing infidelity.

To identify the dominant error sources among the three errors discussed, we run the simulations with each error source over 50 gate durations. This results in the damping of the Rabi oscillations and exponential decay of the SWAP fidelity over a duration of 4 ms, as shown in Fig. 11(d). For phase and intensity errors, each data point is an average of the fidelity over 20 and 25 error pulses, respectively. In agreement with the experimental observations in Ref. [44], we see that interwell hopping is one of the dominant sources of error, whereas phase fluctuations cause the least damping. The larger effect of the intensity error can be explained by the fact that V_s and V_l are the controls for

the optimization, so any variation in them has a significant effect on the fidelity. Note that while the damping of the Rabi oscillations appears similar to the effects caused by decoherence mechanisms such as dephasing and relaxation, our system remains closed even in the presence of additional noise sources. Therefore, in our case, what we refer to as dephasing corresponds to an accumulated coherent gate error rather than interaction with an external environment. The fidelity after one gate duration is greater than 0.998 for all of the error sources. The exponential decay time τ_d is greater than 74 ms, or 460 Rabi oscillations for all errors. This is a predicted improvement of one order of magnitude compared to the experimental decay time $\tau_d = 27$ ms or 33 oscillations [44]. This extended coherence time is primarily due to the shorter gate duration of 0.08 ms compared to the experimental gate duration of 0.4 ms [44].

Result 5. The optimal control pulses are extremely robust against the intensity inhomogeneity, phase fluctuations, and interwell hopping usually appearing in experiments. Interwell hopping is one of the dominant sources of error, whereas phase fluctuations cause the least damping, which agrees with the experimental results [44]. The exponential-decay time τ_d is greater than 460 Rabi oscillations with a gate duration of 0.08 ms, which is an improvement of almost an order of magnitude compared to the experimental τ_d [44].

VIII. FULL GATE OPTIMIZATION WITH HIGHER-BAND FERMİ-HUBBARD MODEL

Recall for the two-band Fermi-Hubbard model from Sec. III B that the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ do not change under SWAP and the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ follow similar dynamics since the Hamiltonian is symmetric. Hence, the optimization for reaching the target state $\Psi_{\text{tar}} = |\downarrow\uparrow\rangle$ also optimizes the full gate, as shown in Fig. 5(a).

Nevertheless, for the higher-band Fermi-Hubbard model, the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ can evolve to other states involving higher levels; e.g., for the four-band Hubbard model, $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ can have six possible states. An efficient SWAP or $\sqrt{\text{SWAP}}$ should maximize the probability of the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ staying in the lowest level at the end of the gate. To check the performance of our optimized controls from Fig. 8, we simulate the system with different initial states and calculate the infidelity of reaching the respective target states using Eq. (13) and the full gate error using Eq. (16) with $N_i = 4$. Figure 12(a) shows the state-evolution errors for different initial states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\rangle$. The states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ have the same errors as in Fig. 8(a) under SWAP gate; however, the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ have significantly higher errors for gate durations shorter than 0.20 ms since the atoms excite to the second level. This results in a full gate error greater than

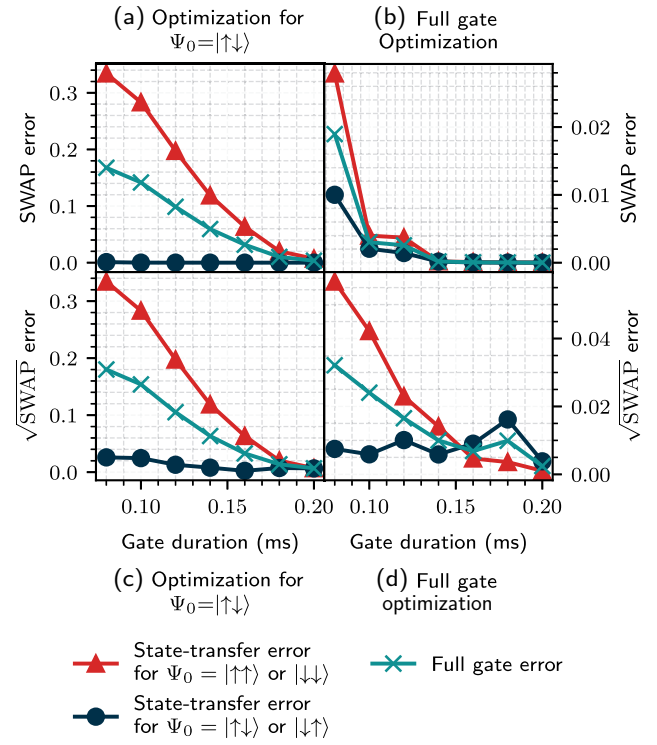


FIG. 12. Comparison of the optimization for one initial state Ψ_0 with the full gate optimization for different gate durations. (a) State-evolution errors for SWAP and different initial states using optimized controls from Fig. 8(a). The initial states $\Psi_{\text{ini}} = |\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ have the same error due to the symmetry of the Hamiltonian, and they have an error of less than 0.001 for gate durations greater than 0.08 ms [same as Fig. 8(a)]. The initial states $\Psi_{\text{ini}} = |\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ also follow the same dynamics but have significantly higher errors for gate durations shorter than 0.20 ms. We show the full gate infidelity calculated with Eq. (16), which is greater than 0.01 for gate durations shorter than 0.20 ms. (b) State evolution for SWAP and different initial states after the full gate optimization with the cost function of Eq. (16). Optimized controls from Fig. 8(a) are used as the initial guess for the full gate optimization. The state-evolution error for $\Psi_{\text{ini}} = |\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ is significantly reduced compared to (a), and we have a full gate error of less than 0.005 for gate durations greater than 0.1 ms. (c) A similar analysis conducted for $\sqrt{\text{SWAP}}$ and different gate durations and controls from Fig. 8(c). (d) The full gate error after further optimization is in the range 0.009–0.001 for gate durations greater than 0.16 ms.

0.01 for gate durations shorter than 0.20 ms. We thus minimize the full gate error by minimizing the cost function defined in Eq. (16) and using the controls from Fig. 8(a) as the initial guess. In Fig. 12(b), we show the state-evolution errors after the full gate optimization. The errors with initial states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are significantly reduced, and we get a full gate error of less than 0.005 for gate durations greater than 0.10 ms.

We perform the same analysis for $\sqrt{\text{SWAP}}$ and calculate the state-evolution error for different initial states, as

shown in Fig. 12(c), using the optimized controls from Fig. 8(c). Similar to the SWAP gate, we see that the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are excited to higher levels, resulting in significant full gate error for gate durations less than 0.20 ms. After optimizing for all four initial states, we can decrease the state-evolution errors and achieve a full gate error of less than 0.009 for gate durations greater than 0.16 ms [see Fig. 12(c)].

Result 6. With the full gate optimization, excitation to the higher bands is minimized for initial states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, and the gate duration is found to be 0.10 ms for the SWAP gate with a fidelity of 0.997 and 0.16 ms for the $\sqrt{\text{SWAP}}$ gate with a fidelity of 0.993.

IX. EFFECT OF HIGH INTERACTION STRENGTH

So far, we have assumed that there are no excitations in the y and z directions of the optical lattice; however, increasing the scattering length a to high values can generate interactions in the y and z directions, resulting in excitations to higher levels. These excitations, if not suppressed, will result in a decrease in gate fidelities. The Hamiltonian for the three-dimensional system is written as

$$H_{3d} = H_J^x \otimes I^y \otimes I^z + I^x \otimes H_E^y \otimes I^z + I^x \otimes I^y \otimes H_E^z + U^x \otimes U^y \otimes U^z, \quad (24)$$

where H_J^x is the hopping plus the onsite energy in the x direction, given by Eqs. (17a) and (17c), H_E^y and H_E^z are onsite energy terms in the y and z directions, respectively, and I is the identity matrix in different directions. Note that there is no hopping in the y and z directions. The interaction term U^x is calculated from the one-dimensional form of Eq. (19), whereas U^y and U^z are calculated from an updated formula given by ($l \in \{y, z\}$)

$$U^l = \int w_m^\dagger(l) w_n^\dagger(l) w_o(l) w_p(l) dl. \quad (25)$$

We consider two energy levels, i.e., $m, n, o, p \in \{0, 1\}$, resulting in four states for each of the y and z directions with two atoms. Combined with the four-band model in the x direction, we have a total of 256 basis states for the three-dimensional simulation using H_{3d} . We simulate the three-dimensional model with optimized controls for different gate durations from Fig. 8(c) and calculate the $\sqrt{\text{SWAP}}$ -gate error. We compare the gate error from the three-dimensional simulation to the four-band one-dimensional model in Fig. 13(a). For a gate duration of 0.12 ms, the infidelity of the $\sqrt{\text{SWAP}}$ gate with the four-band model is 0.007, as shown in Figs. 8(c) and 9(c). The infidelity with the three-dimensional model increases to 0.037 due to small excitations in the y and z directions. In principle, one can make a deeper lattice in the y and z

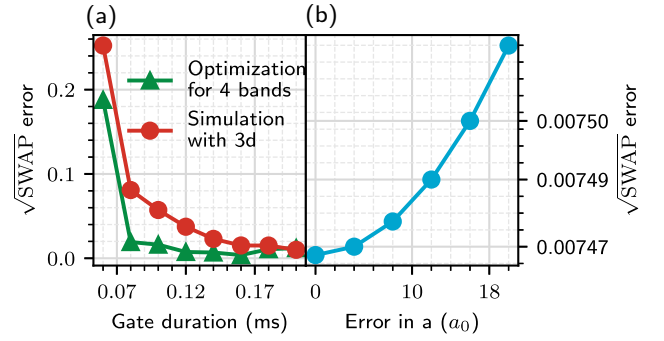


FIG. 13. (a) Comparison of the $\sqrt{\text{SWAP}}$ -gate error between the one-dimensional four-band model and the full three-dimensional simulation for various gate durations. The increase in gate error for the three-dimensional case highlights the effect of excitations in the y and z directions. (b) Robustness analysis of the $\sqrt{\text{SWAP}}$ -gate error against deviations in the scattering length. The gate error remains close to the ideal case for deviations Δa ranging from $4a_0$ to $20a_0$, demonstrating negligible sensitivity of the optimized control pulses (0.12-ms gate duration) to scattering-length deviations.

directions compared to the $45 E_{ry}$ and $45 E_{rz}$ used in our simulations to tightly squeeze the atoms. Additionally, we can perform optimizations to suppress the excitations in these directions.

We optimize the time-independent scattering length a to arbitrary values with respect to an upper bound; however, tuning the magnetic field to achieve the exact a value is difficult. Therefore, we analyze the robustness of the $\sqrt{\text{SWAP}}$ gate against deviations in the scattering length. For this, we simulate the system with the four-band Fermi-Hubbard model using the optimized controls from Fig. 9(a), a 0.12-ms gate duration, and $a = 1995.22 \times a_0$. We take different deviation Δa values from $4a_0$ to $20a_0$, resulting in an effective scattering length of $a + \Delta a$. As shown in Fig. 13(b), the increase in gate error is negligible for this range of deviations, showing the robustness of our optimized pulses.

X. CONCLUSION

Using open-loop quantum optimal control, we design pulses for the SWAP and $\sqrt{\text{SWAP}}$ gates for fermionic atoms trapped in a superlattice reaching fidelities in the range 10^{-3} for realistic experimental parameters. We use Fermi-Hubbard models for the optimization, which widely describe fermionic atoms trapped in optical lattices or superlattices. In this work, we treat the gate optimization as a state-to-state transfer for the SWAP and $\sqrt{\text{SWAP}}$ gates using the two-band Fermi-Hubbard model. Optimizing a SWAP gate thus corresponds to optimizing the transfer of the state $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$. A $\sqrt{\text{SWAP}}$ gate optimization corresponds to optimization of transfer of the state $|\uparrow\downarrow\rangle$ to $[(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$. First, using the two-band

Fermi-Hubbard model, we find the time-optimal control for the SWAP gate analytically and calculate the quantum speed limit in the presence of bounds on the control. We then match the analytical results with numerical optimization of the SWAP gate and show a numerical quantum speed limit closely matching the analytical one under feasibility constraints. We also calculate the full gate fidelities, which is the summation of state-transfer fidelities for all computational states, and we show that the gate fidelities are equivalent to the optimized state-transfer fidelities.

Next, we show the limitations of the two-band Fermi-Hubbard model in the case of fast gates, where it is not sufficient to capture the full dynamics of the double-well system. We describe higher-band Fermi-Hubbard models and update our time-evolution method to account for the nonadiabatic change of the Hamiltonian. We detail a formula to calculate the approximate analytical gradient of the cost function and use a combination of this and the finite-difference method in the optimization. We find that optimization with four bands is sufficient for the SWAP gate, whereas the performance of the $\sqrt{\text{SWAP}}$ gate is further improved by a six-band optimization. Our numerical simulations demonstrate that high-fidelity SWAP and $\sqrt{\text{SWAP}}$ gates can be realized with significantly reduced control durations using realistic experimental parameters. We achieve a SWAP between the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ in 0.08 ms with a fidelity of 0.999, and a $\sqrt{\text{SWAP}}$ pulse preparing the entangled state $[(1+i)|\uparrow\downarrow\rangle - (1-i)|\downarrow\uparrow\rangle]/2$ in 0.12 ms with a fidelity of 0.995, representing a fivefold improvement over experimental state-transfer times [44, 45]. These findings emphasize the potential of higher-band Fermi-Hubbard models for accelerating and optimizing quantum gates.

We test our optimal control pulses for the $\sqrt{\text{SWAP}}$ gate on different atom configurations in the double well. The three- and four-atom error states exhibit significant errors, especially for short gate durations, although these errors can be optimized if necessary. We check the robustness of the optimal control pulses against interwell hopping, phase fluctuations, and intensity inhomogeneity. We show that the optimal pulses are extremely robust against all errors, with inhomogeneous intensity and interwell hopping being the dominant ones. Furthermore, by employing the full gate optimization, we minimize excitations to higher bands for initial states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, achieving a SWAP-gate fidelity of 0.997 in 0.10 ms and a $\sqrt{\text{SWAP}}$ gate fidelity of 0.993 in 0.16 ms. We also explain the different gradient methods used in the paper and compare their performance based on the number of function evaluations and the optimization duration. Our work therefore performs a detailed study of fermionic atoms trapped in a superlattice system and designs faster and more efficient gates. One can also readily adapt the modeling and optimization scheme of this work for bosons by employing the Bose-Hubbard model. Unlike fermions, bosons differ in their interaction energy,

permitting double occupancy by atoms with the same spin states. Furthermore, the creation and annihilation operators for bosons obey the standard commutation relations, in contrast to the fermionic anticommutation relations.

Our optimization model is inspired by experiments and incorporates realistic parameters [44]. The experiments reported in Ref. [44] use phase modulation to perform the SWAP operation, whereas our optimization uses the lattice depths V_s and V_ℓ as the control [45]. This gives the advantage of minimizing the effect of phase noise, which is critical in optical lattice experiments. The pulses generated from optimizing the SWAP and $\sqrt{\text{SWAP}}$ gates are both reasonably smooth and experimentally implementable. Thus, applying these optimized controls to real experiments will enable higher gate fidelities. For more realistic pulses, we can include the transfer-function information in the optimization [106]. The optimized pulses must work with minimal excitation in the y and z directions, which can be achieved with greater y and z lattice depths. Experiments using optimal control will not only enhance gate performance but also enable us to assess and refine our existing models, such as by accounting for heating effects. Moreover, pulses optimized by open-loop approaches are a good starting point for further feedback-based optimizations directly applied in experiments. This iterative approach will pave the way for robust and efficient quantum gates, which are crucial for quantum simulation and computation.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [92].

APPENDIX A: ANALYTICAL SWAP OPTIMIZATION

In this appendix, we find the time-optimal control $J(t)$ and the analytical quantum speed limit for the SWAP gate. We solve the Euler-Lagrange equations for the two-band Fermi-Hubbard model described in Sec. III A. We show

in Sec. II B that for the two-band Fermi-Hubbard model, optimizing the transfer from state $|\uparrow\downarrow\rangle$ to $|\downarrow\uparrow\rangle$ is sufficient to optimize the SWAP gate. As described in Sec. III A, the time evolution with $\tilde{J}(t) = -\sqrt{2}J(t)$ and $U = 0$ is

$$i \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{bmatrix} 0 & 0 & \tilde{J}(t) \\ 0 & 0 & \tilde{J}(t) \\ \tilde{J}(t) & \tilde{J}(t) & 0 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad (\text{A1})$$

where x_1, x_2 , and x_3 correspond to complex coefficients of the states $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$, and $(|D0\rangle + |0D\rangle)/\sqrt{2}$, respectively. Thus, optimizing the SWAP gate reduces to finding $\tilde{J}(t)$ for evolving the system from $(1, 0, 0)^T$ to $(0, 1, 0)^T$, or at least up to a phase factor, as we see below.

With $x_1 = r_1 + ir_4, x_2 = r_2 + ir_5, x_3 = r_6 + ir_3$, and real $r_j = r_j(t)$ and $\tilde{J}(t)$, we obtain

$$\begin{aligned} \dot{r}_1 &= \tilde{J}(t)r_3, \quad \dot{r}_2 = \tilde{J}(t)r_3, \quad \dot{r}_3 = -\tilde{J}(t)r_1 - \tilde{J}(t)r_2, \quad \text{and} \\ \dot{r}_4 &= -\tilde{J}(t)r_6, \quad \dot{r}_5 = -\tilde{J}(t)r_6, \quad \dot{r}_6 = \tilde{J}(t)r_4 + \tilde{J}(t)r_5. \end{aligned}$$

The variables r_1, r_2 , and r_3 are thus decoupled from r_4, r_5 , and r_6 . We obtain two independent three-dimensional subsystems, and we work with the first of these [72]. The ordinary differential equations are given by

$$\begin{pmatrix} \dot{r}_1 \\ \dot{r}_2 \\ \dot{r}_3 \end{pmatrix} = \begin{bmatrix} 0 & 0 & \tilde{J}(t) \\ 0 & 0 & \tilde{J}(t) \\ -\tilde{J}(t) & -\tilde{J}(t) & 0 \end{bmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}. \quad (\text{A2})$$

Clearly, $r_1^2 + r_2^2 + r_3^2 = 1$, provided we start in the subspace r_1, r_2 , and r_3 . From Eq. (A2),

$$\dot{r}_1 = \dot{r}_2 \quad \text{implies} \quad r_1 = r_2 + C \quad (\text{A3})$$

for a suitable real constant C . Minimizing the transfer time T is equivalent [72] to minimizing the functional

$$\mathcal{E} = \int_0^T \tilde{J}^2(t) dt = \int_0^T \mathcal{L} dt,$$

and $\tilde{J}(t) = -\sqrt{2}J(t)$ needs to be bounded for the optimal solution to be well defined. Applying Eq. (A2), the Lagrangian of the system is given by

$$\mathcal{L} = \tilde{J}^2(t) = \frac{\dot{r}_1^2}{r_3^2} = \frac{\dot{r}_1^2}{1 - r_1^2 - r_2^2} = \frac{\dot{r}_1^2}{1 - r_1^2 - (r_1 - C)^2}.$$

The upper bound on the control can be renormalized by the maximum amplitude that is possible in an experiment. We

use the Euler-Lagrange equations

$$\frac{d}{dt} \left[\frac{\partial \mathcal{L}}{\partial \dot{r}_1} \right] = \frac{\partial \mathcal{L}}{\partial r_1} \quad (\text{A4})$$

to find the optimal solution. Computing the left-hand side of Eq. (A4), we have

$$\frac{\partial \mathcal{L}}{\partial \dot{r}_1} = \frac{2\dot{r}_1}{r_3^2} \quad \text{which implies} \quad \frac{d}{dt} \left[\frac{\partial \mathcal{L}}{\partial \dot{r}_1} \right] = 2 \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3^2} \right],$$

and the corresponding right-hand side is given by

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial r_1} &= \frac{\partial}{\partial r_1} \left[\frac{\dot{r}_1^2}{1 - r_1^2 - r_2^2} \right] \\ &= -\frac{\dot{r}_1^2}{(1 - r_1^2 - r_2^2)^2} \frac{\partial}{\partial r_1} [1 - r_1^2 - (r_1 - C)^2] \\ &= \frac{\dot{r}_1^2}{r_3^4} (4r_1 - 2C). \end{aligned}$$

Therefore, Eq. (A4) simplifies to

$$\frac{d}{dt} \left[\frac{\dot{r}_1}{r_3^2} \right] = \frac{\dot{r}_1^2}{r_3^4} (2r_1 - C). \quad (\text{A5})$$

We separately compute

$$\begin{aligned} \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3^2} \right] &= \frac{1}{r_3} \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3} \right] + \frac{\dot{r}_1}{r_3} \frac{d}{dt} \left[\frac{1}{r_3} \right] \\ &= \frac{1}{r_3} \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3} \right] - \frac{\dot{r}_1}{r_3^3} [-\tilde{J}(t)r_1 - \tilde{J}(t)r_2] \\ &= \frac{1}{r_3} \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3} \right] - \frac{\dot{r}_1}{r_3^3} \left[-\frac{\dot{r}_1}{r_3} r_1 - \frac{\dot{r}_1}{r_3} (r_1 - C) \right] \\ &= \frac{1}{r_3} \frac{d}{dt} \left[\frac{\dot{r}_1}{r_3} \right] + \frac{\dot{r}_1^2}{r_3^4} (2r_1 - C), \end{aligned}$$

and we substitute this back into Eq. (A5) to obtain

$$\frac{d}{dt} \left[\frac{\dot{r}_1}{r_3} \right] = 0 = \frac{d\tilde{J}(t)}{dt}.$$

This finally implies that $\tilde{J}(t)$ and $J(t)$ are constant. We substitute $\tilde{J}(t) = -\sqrt{2}A$ in Eq. (A1), where A is a suitable constant. We now consider the initial conditions $x_1(0) = 1, x_2(0) = 0$, and $x_3(0) = 0$. Note that this implies $C = 1$ in Eq. (A3). For these initial conditions, we directly solve Eq. (A1) (which now has only constant coefficients) and obtain

$$x_1 = \cos^2(At), \quad x_2 = -\sin^2(At), \quad x_3 = i \sin(2At)/\sqrt{2}. \quad (\text{A6})$$

For the target state $(0, -1, 0)^T$, we get $AT = \pi/2 + n\pi$. Hence, the fastest transfer from $(1, 0, 0)^T$ to $(0, -1, 0)^T$ can

be attained in a time of $T = \pi/(2A)$. This defines our quantum speed limit for the SWAP gate and is given by the constant hopping parameter $J(t) = A$. Clearly, $J(t) = A$ needs to be bounded by a maximal allowed $J_{\max}$, i.e., $J(t) \leq J_{\max}$. The value of $J_{\max}$ depends on the experimental setup, and we set $J_{\max} = 34.03$ kHz for the two-band numerical simulations in Sec. III B. This means that the quantum speed limit for the two-band SWAP gate is $T = \pi/(2J_{\max})$. We obtain the control $J(t) = A = 34.03$ kHz, and the corresponding quantum speed limit is $T = 0.046$ ms.

APPENDIX B: APPROXIMATE ANALYTICAL GRADIENT

As explained in Sec. V, we cannot use the fast spline-fit method (described in Sec. III B and Appendix C) for calculating the gradients of the cost function C for optimizations using higher-band models. In this appendix, we derive an approximate analytical formula for the gradients and use it in the optimizations performed in Sec. V A. Our primary focus is to find an analytical formula for calculating dC/dV_k , where $V_k \in \{V_s, V_\ell\}$. The cost function C for the target state Ψ_{tar} and the modified time evolution of Eq. (23) is

$$C = 1 - |\langle \Psi_{\text{tar}} | \mathcal{U}_{N_T} \cdot P(w_{t+1}, w_t) \mathcal{U}_t P(w_t, w_{t-1}) \cdot \mathcal{U}_1 | \Psi_{\text{ini}} \rangle|^2.$$

Using the product rule, one infers that dC/dV_k has three terms proportional to $\partial P(w_{t+1}, w_t)/\partial V_k$, $\partial \mathcal{U}_t/\partial V_k$, and $\partial P(w_t, w_{t-1})/\partial V_k$. We approximate the gradient of the unitary evolution operator $\mathcal{U}_t$ as

$$\frac{\partial e^{-iH_t \partial t}}{\partial V_k} = -iH'_t \partial t e^{-iH_t \partial t}, \quad (\text{B1})$$

where H_t is the higher-band Fermi-Hubbard Hamiltonian (17) at time step t . To calculate H'_t from (17), we need to calculate $\partial J_p/\partial V_k$ and $\partial \epsilon_{pm}/\partial V_k$; all other terms proportional to a are zero. The hopping parameter J_p and the onsite energy ϵ_p is calculated from Eqs. (18) and (20), which can also be written as

$$J_p = \frac{E_{2p+1} - E_{2p}}{2}; \quad \epsilon_p = \frac{E_{2p+1} + E_{2p}}{2},$$

where E_j is the energy of the j th band of the double well. Therefore, we can calculate $\partial J_p/\partial V_k$ and $\partial \epsilon_{pm}/\partial V_k$ as

$$\begin{aligned} \frac{\partial J_p}{\partial V_k} &= \frac{1}{2} \left(\frac{\partial E_{2p+1}}{\partial V_k} - \frac{\partial E_{2p}}{\partial V_k} \right), \\ \frac{\partial \epsilon_p}{\partial V_k} &= \frac{1}{2} \left(\frac{\partial E_{2p+1}}{\partial V_k} + \frac{\partial E_{2p}}{\partial V_k} \right). \end{aligned} \quad (\text{B2})$$

Moreover, $\partial E_i/\partial V_k$ can be calculated from

$$\frac{\partial E_i}{\partial V_k} = \sum_j v_{ij}^\dagger \frac{\partial \tilde{H}_1(q)}{\partial V_k} v_{ij}, \quad (\text{B3})$$

where $\tilde{H}_1(q)v_{ij} = E_{ij}v_{ij}$ and $v_{ij}^\dagger v_{ij} = 1$ [110]. Here, $\tilde{H}_1(q)$ denotes the Fourier transform of the Hamiltonian in Eq. (1), and v_{ij} are the eigenstates of $\tilde{H}_1(q)$ [see Sec. II and Eq. (5)]. Thus, we can calculate $\partial \mathcal{U}_t/\partial V_k$ using Eqs. (B1)–(B3), and eventually the final gradient dC/dV_k . Next, the basis-transformation operator $P(w_{t+1}, w_t)$ depends on the Wannier function w_t so that

$$\frac{\partial P(w_{t+1}, w_t)}{\partial V_k} = P \left(w_{t+1}, \frac{\partial w_t}{\partial V_k} \right).$$

The gradient of the Wannier functions is calculated via [110]

$$\frac{\partial w_i}{\partial V_k} = - \sum_j [\tilde{H}_1(q) - E_{ij} \mathcal{I}]^+ \left[\frac{\partial \tilde{H}_1(q)}{\partial V_k} - \frac{\partial E_{ij}}{\partial V_k} \right] v_{ij},$$

where $\mathcal{I}$ is the identity operator and $[\tilde{H}_1(q) - E_{ij} \mathcal{I}]^+$ is the Moore-Penrose inverse of $[\tilde{H}_1(q) - E_{ij} \mathcal{I}]$. The contribution of $\partial P(w_{t+1}, w_t)/\partial V_k$ is negligible in the final gradient dC/dV_k . We thus set this term to zero, speeding up the calculations by avoiding several matrix multiplications. Similarly, we ignore the term $\partial P(w_t, w_{t-1})/\partial V_k$. This approximate analytical gradient computation is significantly faster than the finite-difference method, as shown in Appendix C; however, it becomes difficult to optimize pulses further when we are getting close to the minimum because the approximate analytical method does not provide an exact gradient. Therefore, we reach the minimum SWAP- and $\sqrt{\text{SWAP}}$ -gate error by combining the approximate analytical and finite-difference methods.

APPENDIX C: COMPARISON OF DIFFERENT METHODS TO COMPUTE GRADIENTS

Throughout the paper, we have used gradient-based methods for optimizing the lattice depths V_s and V_ℓ and the scattering length a . We optimize V_s and V_ℓ for the SWAP gate, and V_s , V_ℓ , and a for the $\sqrt{\text{SWAP}}$ gate using GRAPE-like algorithms. The gradient calculation for the optimization of a is trivial, and finite differences work efficiently since we need to optimize only one parameter; however, V_s and V_ℓ are time-dependent and piecewise-constant controls, so we need more sophisticated and faster ways of calculating the gradient. One straightforward way to calculate gradients is to use the finite-difference method to calculate dC/dV_k for $k \in \{s, \ell\}$ at every time step. We use the efficient built-in finite-difference implementation from SCIPY [109] for the comparison in this section. We can also

calculate the gradient analytically using the approximation discussed in Appendix B. For the two-band optimization performed in Sec. III B, we use the spline-fit method to calculate the gradients. For the spline-fit method, we first store a dataset of triples (V_s, V_ℓ, J) . From the stored dataset, we fit a spline function $J = S(V_s, V_\ell)$ over the grid of pairs (V_s, V_ℓ) . We use the SCIPY package [109] for the spline fit, and this function also provides us with the gradient of the estimated J at any pair (V_s, V_ℓ) . We use these gradients in the GRAPE algorithm to run the full optimization (refer to Sec. III B for details). One can also use automatic differentiation for gradient calculation [111], but it can be slow in the presence of multiple matrix diagonalizations for calculating the Wannier states. Hence, we do not analyze the performance of automatic differentiation here. Two parameters are used to test the efficiency of different gradient methods. First, we check the number of cost-function evaluations in the optimization for a particular gradient method. Secondly, the total optimization run times are compared for different gradients.

We compare the gradient methods for the two-band model at varying gate durations. Figure 14(a) shows that the finite-difference method results in the highest number of function evaluations for every gate duration, whereas the approximate analytical and spline-fit methods are comparable. Function evaluations decrease for longer gate durations due to lower initial gate error and easier optimization tasks for longer durations. Figure 14(b) provides insights into the performance of different gradient methods. The finite-difference method is the slowest to reach the minima, and optimization times increase linearly with the gate duration. The approximate analytical and spline-fit methods result in run times that are relatively independent of the gate duration; however, the approximate analytical gradient requires a longer time compared to the spline fit. As the spline fit calculates J and dC/dV_k from existing fitted functions, it avoids several matrix diagonalizations and multiplications needed for calculating the Wannier states, which make the approximate analytical gradient computationally more expensive.

A similar comparison is conducted for the four-band model, where we compare the performance of the approximate analytical gradient with the finite-difference gradient. Note that since we have to calculate basis-transformation operators at every time step, we cannot use the spline-fit method for higher-band optimization. We set an upper bound on the number of function evaluations for both the finite-difference method and the approximate analytical method. As we can see in Fig. 14(c) both methods have maximal function evaluations for all gate durations; however, finite differences lead to longer optimization times when compared to the approximate analytical method as shown in Fig. 14(d). This suggests that the spline-fit method performs significantly better than the approximate analytical and finite-difference methods, but for higher

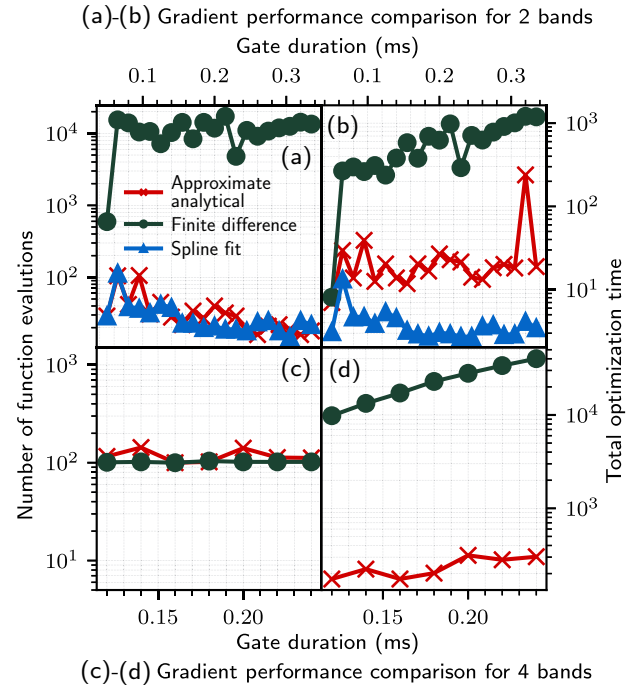


FIG. 14. Performance of the approximate analytical, finite-difference, and spline methods for computing the gradient for (a),(b) two-band and (c),(d) four-band Fermi-Hubbard optimizations: (a),(b) Overall, the spline method performs best both in the number of evaluations and the total optimization time, remaining mostly constant regardless of the gate duration, while the finite-difference method performs worst, and its total optimization time increases with the gate duration. (c),(d) The number of function evaluations for the approximate analytical gradient computation is comparable to the finite-difference method, which, however, performs much worse for the total optimization time. The spline method is not available for four bands.

bands, we cannot use the spline-fit method. In that case, the use of approximate analytical gradients is computationally effective; however, since the approximate analytical method does not give an exact gradient, we use a combination of the approximate analytical and finite-difference methods to minimize the cost function in Sec. V A. Hence, we use multiple methods for gradient calculation depending on the complexity of the system. Different methods have different trade-offs, and combining them enables fast and efficient optimizations.

APPENDIX D: ASSIGNMENT OF COMPUTATIONAL BASIS

In this appendix, we describe the method used for finding computational basis states and labeling them for different numbers of atoms in a double well. We use this labeling method in Sec. VI to simulate the dynamics of different atom configurations. Suppose we have M levels and N atoms in the double well. Since each level consists of the left and right sides of the double well, we have a

TABLE II. Scheme explaining the calculation and labeling of the computational states for $N_\uparrow = 1$ and $N_\downarrow = 1$. In the first column, the total number of bits is the number of sites, and the number of 1s in each bit configuration represents the number of spins up. The same applies to the second column, where spins up are replaced with spins down. The states are ordered first by spin up (first and third columns) and then by spin down (second and fourth columns). The final label (fifth column) is computed from Eq. (D1).

$\uparrow$	$\downarrow$	$I_\uparrow$	$I_\downarrow$	$I = I_\uparrow \binom{S}{N_\uparrow} + I_\downarrow$
0001	0001	0	0	0
0001	0010	0	1	1
:	:	:	:	:
0010	0001	1	0	4
:	:	:	:	:
1000	1000	3	3	15

total of $S = 2 \times M$ sites. Now suppose we have $N_\uparrow$ atoms with spin up and $N_\downarrow$ with spin down, i.e., $N = N_\uparrow + N_\downarrow$. We can arrange $N_\uparrow$ identical spin-up fermionic atoms in $\binom{S}{N_\uparrow} = S!/N_\uparrow!(S - N_\uparrow)!$ ways in S sites. For each configuration of the spin-up atoms, we can arrange the spin-down atoms in $\binom{S}{N_\downarrow} = S!/N_\downarrow!(S - N_\downarrow)!$ ways. The total number of possibilities to arrange $N = N_\uparrow + N_\downarrow$ atoms in a double well is the number of computational states and is given by $N_B = \binom{S}{N_\uparrow} \times \binom{S}{N_\downarrow}$. As an example, Table II shows the possible computational basis states for two atoms with one spin-up atom and one spin-down atom used in the four-band Fermi-Hubbard model in Sec. V. Here, $M = 2$, $S = 4$, $N = 2$, $N_\uparrow = 1$, and $N_\downarrow = 1$. Therefore, the total number of computational states is 16. We represent the spin-up and spin-down states by S bits and label our computational state using the following formula:

$$I = I_\uparrow \binom{S}{N_\uparrow} + I_\downarrow, \quad (\text{D1})$$

where these values satisfy $I_\uparrow \in \{0, \dots, \binom{S}{N_\uparrow} - 1\}$, $I_\downarrow \in \{0, \dots, \binom{S}{N_\downarrow} - 1\}$, and $I \in \{0, \dots, N_B - 1\}$.

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